10/560,577

[redacted] 12/10/2004

=> d que l33
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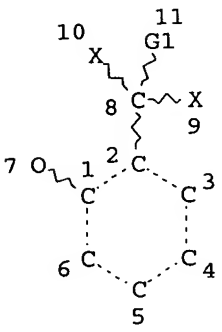

VAR G1=H/X/12
NODE ATTRIBUTES:
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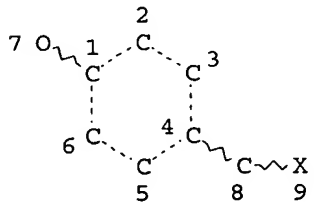
CONNECT IS E3 RC AT 4
CONNECT IS E2 RC AT 5
CONNECT IS E2 RC AT 6
CONNECT IS E2 RC AT 7
CONNECT IS E1 RC AT 12
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE
L9 3146 SEA FILE=REGISTRY SSS FUL L7
L15 STR



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CONNECT IS E2 RC AT 7
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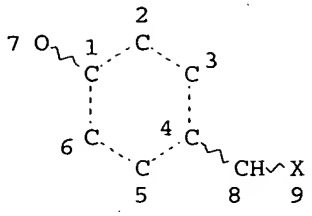
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE

L17 4953 SEA FILE=REGISTRY SSS FUL L15
L18 STR



NODE ATTRIBUTES:
CONNECT IS E2 RC AT 2
CONNECT IS E2 RC AT 3
CONNECT IS E2 RC AT 5
CONNECT IS E2 RC AT 6
CONNECT IS E2 RC AT 7
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE
L19 1145 SEA FILE=REGISTRY SUB=L17 SSS FUL L18
L20 4291 SEA FILE=REGISTRY ABB=ON PLU=ON L9 OR L19
L24 102 SEA FILE=REGISTRY ABB=ON PLU=ON CYANINE?/CN
L25 464 SEA FILE=REGISTRY ABB=ON PLU=ON FLUORESCEIN?/CN
L26 640 SEA FILE=REGISTRY ABB=ON PLU=ON BIOTIN?/CN
L27 7 SEA FILE=REGISTRY ABB=ON PLU=ON SULFORHODAMINE?/CN
L28 8 SEA FILE=REGISTRY ABB=ON PLU=ON TETRAMETHYLRHODAMINE?/CN
L29 16 SEA FILE=REGISTRY ABB=ON PLU=ON DINITROPHENYL?/CN
L30 1237 SEA FILE=REGISTRY ABB=ON PLU=ON (L24 OR L25 OR L26 OR L27 OR L28 OR L29)
L31 147720 SEA FILE=HCAPLUS ABB=ON PLU=ON DYES+PFT,NT,RTCS/CT
L32 189010 SEA FILE=HCAPLUS ABB=ON PLU=ON L30 OR L31
L33 21 SEA FILE=HCAPLUS ABB=ON PLU=ON L20 AND L32

=> d l33 ibib abs hitind hitstr 1-21

L33 ANSWER 1 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2004:142963 HCAPLUS
DOCUMENT NUMBER: 140:199334
TITLE: Preparation of 2,4-pyrimidinediamines as IgE and/or IgG receptor modulators for treatment of autoimmune diseases
INVENTOR(S): Singh, Rajinder; Argade, Ankush; Payan, Donald G.; Clough, Jeffrey; Keim, Holger; Sylvain, Catherine; Li, Hui; Bhamidipati, Somasekhar
PATENT ASSIGNEE(S): Rigel Pharmaceuticals, USA
SOURCE: PCT Int. Appl., 811 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004014382	A1	20040219	WO 2003-US24087	20030729

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

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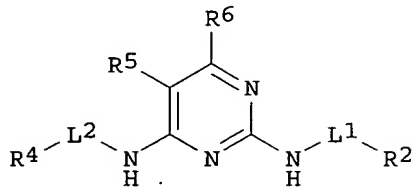
PRIORITY APPLN. INFO.:		
US 2002-399673P	P	20020729
US 2003-443949P	P	20030131
US 2003-452339P	P	20030306
US 2003-631029	A	20030729

OTHER SOURCE(S): MARPAT 140:199334

GI



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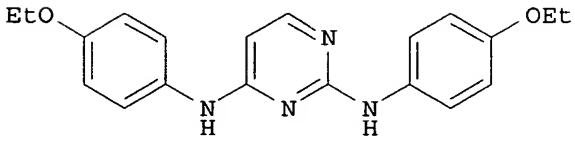

II

AB The present invention provides methods of treating or preventing autoimmune diseases with 2,4-pyrimidinediamine compds., as well as methods of treating, preventing or ameliorating symptoms associated with such diseases. Title compds. I [wherein L1 and L2 = independently a bond or a linker; R2 = (un)substituted alkyl, (hetero)cycloalkyl, or (hetero)aryl; R4 = H or R2; R5 = R6 or (un)substituted alkyl, alkenyl, or alkynyl; R6 = independently H, an electroneg. group, protected alc. or thiol, haloalkyl(oxy), halo, CN, NC, OCN, SCN, NO, NO2, N3, or (un)substituted amino, sulfamoyl(oxy), acyl, carboxy, carbamoyl, (hetero)aryl(alkyl), etc.; with provisos and exclusions; and salts, hydrates, solvates, N-oxides, and prodrugs thereof] were prepared as inhibitors of the IgE and/or IgG receptor signaling cascades that lead to the release of chemical mediators. For example, coupling of 2,4-dichloropyrimidine with 4-ethoxyaniline in EtOH provided N2,N4-bis(4-ethoxyphenyl)-2,4-pyrimidinediamine (II). The latter inhibited degranulation of bone marrow derived mast cells challenged with anti-IgE and ionomycin with IC50 values of 4.5 μM and 4.4 μM, resp. Thus, I and their pharmaceutical compns. are useful in the treatment and prevention of diseases

characterized by, caused by, or associated with the release of chemical mediators via degranulation of mast, basophil, neutrophil, or eosinophil cells and other processes effected by activation of the IgE and/or IgG receptor signaling cascades. Specific examples of autoimmune diseases that can be treated or prevented with I and their pharmaceutical compns. include rheumatoid arthritis, systemic lupus erythematosis, and multiple sclerosis (no data).

IC ICM A61K031-506
ICS A61K031-519

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

IT

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575477-41-7P	575477-42-8P			

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(IgE and/or IgG receptor modulator; preparation of pyrimidinediamines as IgE and/or IgG receptor modulators for treatment of autoimmune diseases)

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575484-33-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(IgE and/or IgG receptor modulator; preparation of pyrimidinediamines as IgE and/or IgG receptor modulators for treatment of autoimmune diseases)

IT 51-06-9 51-21-8, 5-Fluorouracil 51-67-2, Tyramine 54-20-6,

5-Trifluoromethyluracil 55-81-2, 2-(4-Methoxyphenyl)ethylamine 56-41-7, L-Alanine, reactions **58-85-5**, D-(+)-Biotin 61-54-1, Tryptamine 64-04-0, 2-Aminoethylbenzene 65-49-6, 4-Amino-2-hydroxybenzoic acid 67-64-1, Acetone, reactions 75-31-0, Isopropylamine, reactions 77-92-9, Citric acid, reactions 78-96-6, 2-Hydroxypropylamine 88-19-7 89-57-6, 5-Amino-2-hydroxybenzoic acid 90-41-5, 2-Phenylaniline 91-00-9, 1,1-Diphenylmethylamine 95-76-1, 3,4-Dichloroaniline 95-80-7 96-32-2, Methyl bromoacetate 96-97-9, 2-Hydroxy-5-nitrobenzoic acid 98-16-8, 3-Trifluoromethylaniline 98-80-6, Phenylboronic acid 99-03-6, 3-Methylcarbonylaniline 99-05-8, 3-Aminobenzoic acid 99-09-2, 3-Nitroaniline 99-53-6 99-55-8, 2-Methyl-5-nitroaniline 99-57-0, 2-Amino-4-nitrophenol 99-59-2, 2-Methoxy-5-nitroaniline 99-88-7, 4-Isopropylaniline 99-98-9 100-02-7, 4-Nitrophenol, reactions 100-15-2, N-Methyl-4-nitroaniline 102-28-3 102-50-1, 4-Methoxy-2-methylaniline 103-71-9, Phenyl isocyanate, reactions 104-78-9, 3-(Diethylamino)propylamine 104-94-9, 4-Methoxyaniline 105-36-2, Ethyl bromoacetate 106-47-8, 4-Chloroaniline, reactions 106-49-0, 4-Methylaniline, reactions 106-50-3, 1,4-Diaminobenzene, reactions 107-10-8, n-Propylamine, reactions 107-11-9, Allylamine 108-42-9, 3-Chloroaniline 108-45-2, 3-Aminoaniline, reactions 108-91-8, Cyclohexylamine, reactions 109-01-3, N-Methylpiperazine 109-73-9, n-Butylamine, reactions 109-76-2, 1,3-Diaminopropane 109-81-9 109-83-1, N-Methyl-N-2-hydroxyethylamine 109-85-3, 2-Methoxyethylamine 109-90-0, Ethyl isocyanate 110-15-6, Succinic acid, reactions 110-16-7, Maleic acid, reactions 110-17-8, Fumaric acid, reactions 110-85-0, Piperazine, reactions 110-89-4, Piperidine, reactions 110-91-8, Morpholine, reactions 111-42-2, reactions 116-09-6 119-32-4, 4-Methyl-3-nitroaniline 121-90-4, 3-Nitrobenzoyl chloride 122-80-5, 4-Acetamidoaniline 123-30-8, 4-Hydroxyaniline 123-75-1, Pyrrolidine, reactions 124-68-5, 2-Amino-2-methylpropanol 135-95-5, 3-Hydroxymethyl-4-methoxyaniline 136-17-4 139-59-3, 4-Phenoxyaniline 141-86-6, 2,6-Diaminopyridine 150-13-0, 4-Aminobenzoic acid 156-43-4, 4-Ethoxyaniline 156-87-6, 3-Hydroxypropylamine 320-51-4, 4-Chloro-3-trifluoromethylaniline 349-55-3, 3-Methoxy-5-trifluoromethylaniline 364-76-1, 4-Fluoro-3-nitroaniline 367-21-5, 3-Chloro-4-fluoroaniline 368-53-6 369-36-8, 2-Fluoro-5-nitroaniline 369-68-6, 3-(Trifluoromethylthio)aniline 371-40-4, 4-Fluoroaniline 372-16-7, 4-(Trifluoromethylthio)aniline 372-19-0, 3-Fluoroaniline 372-39-4, 3,5-Difluoroaniline 399-95-1, 2-Fluoro-4-hydroxyaniline 399-96-2, 3-Fluoro-4-hydroxyaniline 403-40-7, 4-Fluoro-α-methylbenzylamine 452-69-7, 4-Fluoro-3-methylaniline 452-84-6, 2-Fluoro-5-methylaniline 454-67-1, 3-Amino-5-fluorobenzotrifluoride 455-14-1, 4-Trifluoromethylaniline 459-73-4, Ethyl 2-aminoacetate 461-82-5, 4-Trifluoromethoxyaniline 462-08-8, 3-Aminopyridine 492-41-1, (1R,2S)-(-)-Norephedrine 501-53-1, Benzyl chloroformate 505-66-8, Homopiperazine 513-37-1, 1-Chloro-2-methylpropene 534-03-2, 2-Amino-1,3-propanediol 536-90-3, 3-Methoxyaniline 539-74-2, Ethyl 3-bromopropionate 540-51-2, 1-Bromo-2-hydroxyethane 554-84-7, 3-Nitrophenol 580-15-4, 6-Aminoquinoline 582-33-2, 3-Ethoxycarbonylaniline 589-16-2, 4-Ethylaniline 591-27-5, 3-Hydroxyaniline 593-51-1, Methylamine hydrochloride 600-00-0 611-08-5, 5-Nitrouracil 616-30-8, 3-Amino-1,2-propanediol 617-89-0, Furfurylamine 619-08-9, 2-Chloro-4-nitrophenol 621-33-0, 3-Ethoxyaniline 623-04-1, 4-Aminobenzyl alcohol 623-33-6, Glycine ethyl ester hydrochloride 626-43-7, 3,5-Dichloroaniline 634-93-5, 2,4,6-Trichloroaniline 635-21-2, 2-Carboxy-4-chloroaniline 635-22-3, 4-Chloro-3-nitroaniline 695-34-1, 2-Amino-4-methylpyridine 720-01-4 765-30-0, Cyclopropylamine 765-39-9, 1-Aminopyrrole 769-92-6,

4-tert-Butylaniline 873-74-5, 4-Aminobenzonitrile 1009-36-5,
4-Chloro-3-methoxynitrobenzene 1072-98-6, 5-Chloro-2-aminopyridine
1080-06-4, L-Tyrosine methyl ester 1118-68-9, N,N-Dimethylglycine
1193-21-1, 4,6-Dichloropyrimidine 1462-37-9, 1-Benzyloxy-2-bromoethane
1476-23-9, Allyl isocyanate 1484-26-0, 3-Benzyloxyaniline 1535-73-5,
3-Trifluoromethoxyaniline 1535-76-8 1544-85-0 1603-41-4,
5-Methyl-2-aminopyridine 1673-47-8, 3-Chlorobenzohydrazide 1679-18-1,
4-Chlorophenylboronic acid 1687-53-2, 3-Hydroxy-4-methoxyaniline
1780-31-0, 2,4-Dichloro-5-methylpyrimidine 1780-40-1,
2,4,5,6-Tetrachloropyrimidine 1795-48-8, Isopropyl isocyanate
1798-11-4, 4-Nitrophenoxyacetic acid 1822-94-2, 5-(Chloromethyl)-3-
phenyl-1,2,4-oxadiazole 1824-81-3, 2-Amino-6-methylpyridine 1877-77-6,
3-Aminobenzyl alcohol 1949-55-9 2038-03-1, 4-Morpholineethanamine
2106-50-5, 2-Chloro-4-fluoronitrobenzene 2144-37-8, Methyl
5-(chloromethyl)-2-furoate 2216-51-5 2237-30-1, 3-Aminobenzonitrile
2243-47-2, 3-Phenylaniline 2393-17-1, 3-(p-Aminophenyl)propionic acid
2393-23-9, 4-Methoxybenzylamine 2423-71-4, 2,6-Dimethyl-4-nitrophenol
2516-34-9, Cyclobutylamine 2516-47-4, Cyclopropylmethylamine 2524-67-6
2597-56-0, 2-Methoxy-4-nitrobenzoic acid 2620-50-0, Piperonylamine
2627-86-3 2666-93-5, Leucine methyl ester 2735-04-8,
2,4-Dimethoxyaniline 2743-60-4, L-Leucine ethyl ester 2835-68-9
2835-78-1, 3-Phenylcarbonylaniline 2835-95-2, 3-Hydroxy-4-methylaniline
2835-96-3, 4-Hydroxy-3-methylaniline 2836-04-6, 3-(Dimethylamino)aniline
2949-22-6 3081-24-1 3096-69-3, 2,3-Dimethyl-4-hydroxyaniline
3096-71-7, 2,5-Dimethyl-4-hydroxyaniline 3182-93-2, L-Phenylalanine
ethyl ester hydrochloride 3343-28-0, N-Phthaloyl-DL-glutamic anhydride
3544-25-0, 4-Cyanomethylaniline 3665-80-3, N-Ethyl-4-nitroaniline
3676-85-5, 4-Aminophthalimide 3731-51-9, 2-Pyridylmethylamine
3731-52-0, 3-Pyridylmethylamine 3764-01-0, 2,4,6-Trichloropyrimidine
3863-11-4, 3,4-Difluoroaniline 3886-69-9 3934-20-1,
2,4-Dichloropyrimidine 3964-52-1, 3-Chloro-4-hydroxyaniline 4152-09-4,
N-Benzyl-1,2-diaminoethane 4344-55-2, 4-Butoxyaniline 4403-70-7,
3-Aminobenzylamine 4425-56-3, 5-Cyanouracil 4442-59-5,
2,3-Dihydro-1,4-benzodioxin-2-ylmethylamine 4461-30-7 4487-59-6,
2-Bromo-5-nitropyridine 4543-47-9, 3-Furanmethanamine 4553-21-3
4747-71-1, Cyclopentyl isocyanate 5061-21-2 5071-96-5,
3-Methoxybenzylamine 5131-58-8 5192-03-0, 5-Aminoindole 5228-48-8
5292-43-3, tert-Butyl bromoacetate 5318-27-4, 6-Aminoindole 5345-54-0,
3-Chloro-4-methoxyaniline 5350-93-6 5369-16-4, 3-Isopropylaniline
5369-19-7, 3-tert-Butylaniline 5401-94-5 5428-54-6,
2-Methyl-5-nitrophenol 5438-70-0, Ethyl 4-aminophenyl acetate
5445-26-1, Ethyl 4-nitrophenylacetate 5683-33-0 5862-77-1,
3-Amino-4-ethoxyaniline 5930-28-9, 3,5-Dichloro-4-hydroxyaniline
5978-75-6, 9-Aminofluorene hydrochloride 6264-67-1 6269-89-2,
1-(4-Nitrophenyl)piperazine 6299-85-0 6315-89-5, 3,4-Dimethoxyaniline
6358-64-1, 2,5-Dimethoxy-4-chloroaniline 6421-88-1 6628-77-9,
3-Amino-6-methoxypyridine 6967-12-0, 6-Aminoindazole 7568-93-6,
2-Amino-1-phenylethanol 7597-18-4 7647-01-0, Hydrochloric acid,
reactions 7664-66-6, 4-Isopropoxyaniline 10242-12-3,
5-Nitro-2-benzofurancarboxylic acid 10272-07-8, 3,5-Dimethoxyaniline
13331-23-2, Furan-2-boronic acid 13871-68-6, 4-Acetoxyaniline
14268-66-7, 3,4-Methylenedioxyaniline 14415-44-2, 6-Aminocoumarin
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrimidinediamines as IgE and/or IgG receptor modulators for
treatment of autoimmune diseases)

IT 14576-22-8 16154-69-1, 4-(4-Benzylpiperazin-1-yl)aniline 16452-01-0,
3-Methoxy-4-methylaniline 16642-79-8, 3-(p-Nitrophenyl)propionic acid
16732-57-3 17413-10-4 17431-03-7, L-Valine ethyl ester 17742-69-7,
3,5-Dichloro-4-methoxynitrobenzene 19293-62-0 19335-11-6,

5-Aminoindazole 19617-43-7, Ethoxycarbonyl isocyanate 20348-09-8, 2H-Pyrido[3,2-b]-1,4-oxazin-3(4H)-one 20439-47-8, (R,R)-1,2-Diaminocyclohexane 20734-67-2, 5-Aminobenzene-1,3-diol 21169-65-3 21443-96-9, 7-Aminoindazole 22013-33-8, 3,4-Ethylenedioxyaniline 22038-86-4, (R)-(+)-1-(4-Methoxyphenyl)ethylamine 22235-25-2, 3-Methoxycarbonyl-5-trifluoromethylaniline 24313-88-0, 3,4,5-Trimethoxyaniline 24358-62-1, 1-(4-Bromophenyl)ethylamine 24424-99-5, Di-tert-butyl dicarbonate 25170-72-3 26215-14-5 26682-99-5, Phenylglycine methyl ester 27906-24-7 28020-37-3, 3-Amino-2,6-dimethoxypyridine 28059-69-0 28485-17-8, 5-Ethoxycarbonyluracil 28942-84-9 29263-94-3, Diethyl 2-bromo-2-methylmalonate 30418-59-8, 3-Aminophenylboronic acid 30734-81-7 30866-24-1 31329-64-3 33311-29-4 33786-89-9, 3-Amino-5-chloroaniline 33901-46-1 36082-50-5, 5-Bromo-2,4-dichloropyrimidine 36946-70-0, 2-Aminoindole 37045-73-1, 3-Methylsulfonylaminoaniline 38560-96-2, 4-Chloro-3,5-dimethylnitrobenzene 38910-17-7 39811-17-1, 2-Methoxy-5-phenylaniline 39905-57-2, 4-n-Hexyloxyaniline 40353-34-2, 7-Nitro-1-tetralone 40615-04-1, Benzo[b]thiophene-3-methanamine 41402-58-8 41406-00-2, 3-Isopropoxyaniline 41851-59-6, (S)-(-)-1-(4-Methoxyphenyl)ethylamine 42758-84-9, 3-Acetoxyaniline 42923-79-5 42933-43-7, 5-Amino-2,3-dihydrobenzofuran 42961-88-6 50541-93-0, N-Benzyl-4-aminopiperidine 50593-24-3 50868-72-9, 5-Methoxy-2-methylaniline 50963-77-4 52481-41-1 52547-48-5 52913-11-8 53222-92-7 53250-82-1 54368-61-5 54962-75-3, 3-Bromo-5-trifluoromethylaniline 55411-44-4, 4-Amino-2-chloro-6-methylphenol 55745-74-9 56607-76-2 56813-48-0 56932-44-6 56970-26-4, 4-Methoxy-3-phenylaniline 57319-65-0 57946-65-3 58754-71-5, 4-(2,3-Dihydroxypropoxy)aniline 59404-86-3 59954-04-0, Methyl 4-aminophenoxyacetate 62345-76-0 62802-42-0, 2-Chloro-5-fluoropyrimidine 63503-60-6, 3-Chlorophenylboronic acid 64628-73-5, 3-Chloro-4-trifluoromethoxyaniline 65934-74-9, 4-Methyl-3-trifluoromethylaniline 66211-46-9, (R)-3-Amino-1,2-propanediol 67952-93-6, 3-Chloro-4-methylbenzylamine 68621-88-5, 3-tert-Butoxycarbonylaminoaniline 69411-68-3, 3-Fluoro-4-trifluoromethylaniline 69959-88-2 70264-94-7, Methyl (4-bromomethyl)-3-methoxybenzoate **70338-47-5**, 4-Benzyloxy-3-trifluoromethylaniline 71026-66-9, 4-tert-Butoxycarbonylaminoaniline 71056-61-6 71597-85-8, 4-Hydroxyphenylboronic acid 73246-45-4, Methyl (S)-(-)-2-chloropropionate 73732-51-1, 3-(Tetrazol-5-yl)aniline 76445-65-3, 4-Aminocyclohexanol hydrochloride 77287-29-7, Methyl (R)-(+)-2-chloropropionate 80938-67-6 81720-19-6 87029-84-3 88327-91-7, 4-(Tetrahydro-(1H)-pyrrol-1-ylsulfonyl)aniline 89260-46-8 89586-07-2 89976-75-0 92028-21-2 94838-55-8 94839-07-3, 3,4-Methylenedioxyphenylboronic acid 96100-12-8 98280-30-9 99768-12-4, (4-Methoxycarbonylphenyl)boronic acid 100800-40-6, 4-[[3-(N-Morpholino)propyl]oxy]aniline 103361-43-9 105807-84-9, 6-Amino-2,2-dimethyl-4H-benzo[1,4]oxazin-3-one 108761-82-6 110178-35-3 126874-73-5 134855-87-1, 1-(4-Hydroxyphenyl)ethylamine 136544-55-3 141068-81-7 143071-39-0, 2-(2-Hydroxyethoxy)-5-nitropyridine 157837-31-5, 3-(1,3-Oxazol-5-yl)aniline 158196-47-5 167027-30-7 167756-90-3, 3-((N-tert-Butoxycarbonyl-N-methylamino)methyl)aniline 169286-84-4 173735-84-7 175136-34-2 175137-27-6 175201-62-4 175205-10-4 180258-45-1 189683-22-5 194025-85-9, 3-Methylaminocarbonyl-4-methoxyaniline 195046-11-8 203664-68-0 203664-71-5 205117-39-1 205672-25-9 206761-76-4 209899-47-8, 3-[(N-tert-Butoxycarbonyl)aminomethyl]-4-methylaniline 220844-82-6 226571-61-5 280581-65-9 306934-74-7 306934-85-0 306937-22-4, Ethyl 1-(3-aminobenzyl)piperidine-4-carboxylate 307989-43-1

337463-65-7 439095-26-8 503166-47-0, 3-(N-Morpholinomethyl)-4-methoxyaniline 575472-85-4 575472-93-4, 2H-1,4-Benzoxazin-6-amine
575472-98-9 575473-25-5, 5-Amino-1-methylindazoline 575473-51-7
575473-75-5 575473-89-1 575473-93-7 575473-95-9 575473-97-1
575474-01-0 575474-14-5, 4H-Imidazo[2,1-c][1,4]benzoxazin-8-amine
575474-23-6 575474-31-6 575474-41-8 575476-29-8 575476-87-8
575476-92-5 575477-07-5 575477-12-2 575477-14-4 575477-17-7
575477-26-8 575477-29-1 575477-33-7 575477-51-9 575477-68-8
575477-86-0 575478-04-5 575478-14-7 575478-36-3 575478-38-5
575478-41-0 575478-52-3 575478-54-5 575478-60-3 575478-64-7
575478-68-1 575478-73-8 575478-82-9 575478-83-0 575478-85-2
575479-04-8 575479-26-4 575479-32-2 575479-34-4 575479-45-7
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575479-98-0 575480-00-1 575480-04-5 575480-11-4 575480-13-6
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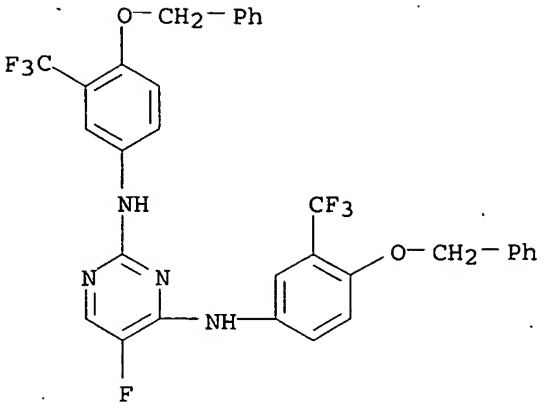
575480-47-6 575480-51-2 575480-76-1 575480-83-0 575480-85-2
575480-93-2 575481-41-3 575481-44-6 575481-48-0 575481-53-7
575481-61-7 575481-66-2 575481-69-5 575481-71-9 575481-73-1
575481-75-3 575481-77-5 575481-86-6 575481-92-4 575481-94-6
575482-11-0 575482-16-5 575482-18-7 575482-40-5 575482-50-7
575482-55-2 575482-60-9 575482-69-8 575482-84-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrimidinediamines as IgE and/or IgG receptor modulators for treatment of autoimmune diseases)

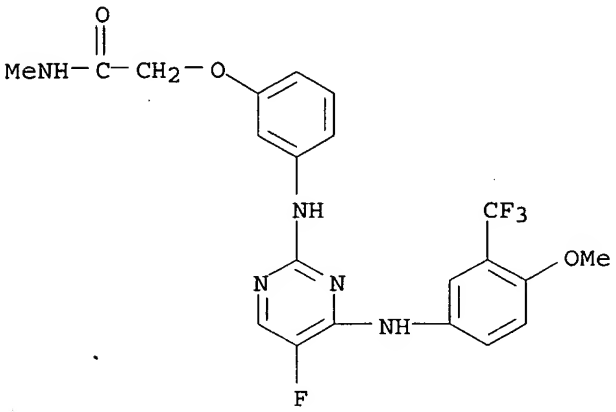
IT 575482-89-2 575482-92-7 575482-94-9 575482-96-1 **575482-98-3**
575483-00-0 575483-03-3 575483-08-8 575483-11-3 575483-19-1
575483-62-4 575483-70-4 575483-77-1 575483-89-5 575483-91-9
575484-00-3 575484-02-5 575484-23-0 575484-55-8 575484-63-8
575484-64-9 575484-66-1 575484-71-8 575484-74-1 575484-83-2
575485-07-3 575485-10-8 575485-12-0 575485-27-7 575485-38-0
575485-43-7 575485-61-9 575485-66-4 575486-13-4 575486-31-6
575486-34-9 575486-37-2 575486-42-9 575486-45-2 575487-16-0
662228-28-6 662228-35-5 662245-28-5 662245-63-8 662245-76-3
662245-79-6 662246-48-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrimidinediamines as IgE and/or IgG receptor modulators for treatment of autoimmune diseases)

IT **575476-23-2P 575482-97-2P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(IgE and/or IgG receptor modulator; preparation of pyrimidinediamines as IgE and/or IgG receptor modulators for treatment of autoimmune diseases)

RN 575476-23-2 HCAPLUS
CN 2,4-Pyrimidinediamine, 5-fluoro-N,N'-bis[4-(phenylmethoxy)-3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

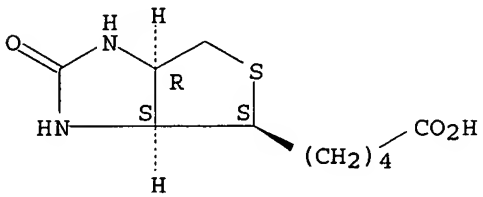


RN 575482-97-2 HCAPLUS
CN Acetamide, 2-[3-[[5-fluoro-4-[[4-methoxy-3-(trifluoromethyl)phenyl]amino]-2-pyrimidinyl]amino]phenoxy]-N-methyl- (9CI) (CA INDEX NAME)



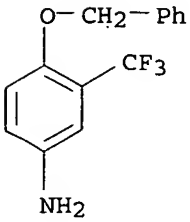
IT **58-85-5**, D-(+)-Biotin **70338-47-5**, 4-Benzyloxy-3-trifluoromethylaniline **575482-98-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrimidinediamines as IgE and/or IgG receptor modulators for treatment of autoimmune diseases)
RN 58-85-5 HCAPLUS
CN 1H-Thieno[3,4-d]imidazole-4-pentanoic acid, hexahydro-2-oxo-, (3aS,4S,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

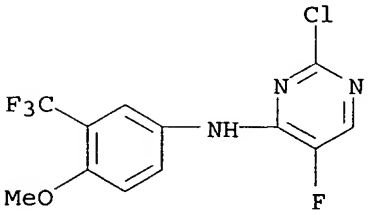


RN 70338-47-5 HCAPLUS

CN Benzenamine, 4-(phenylmethoxy)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 575482-98-3 HCAPLUS
CN 4-Pyrimidinamine, 2-chloro-5-fluoro-N-[4-methoxy-3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 2 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:950982 HCAPLUS
DOCUMENT NUMBER: 140:16736
TITLE: Preparation of diarylurea derivatives useful for the treatment of protein kinase dependent diseases
INVENTOR(S): Floersheimer, Andreas; Furet, Pascal; Manley, Paul William; Bold, Guido; Boss, Eugen; Guagnano, Vito; Vaupel, Andrea
PATENT ASSIGNEE(S): Novartis A.-G., Switz.; Novartis Pharma G.m.b.H.
SOURCE: PCT Int. Appl., 170 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

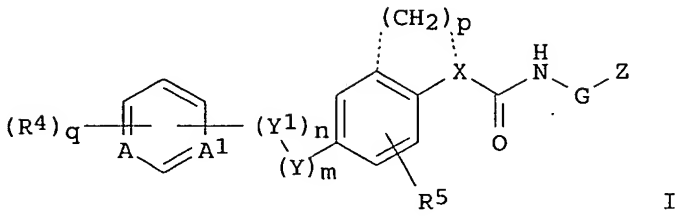
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003099771	A2	20031204	WO 2003-EP5634	20030528
WO 2003099771	A3	20040401		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LT, LU, LV, MA, MD, MK, MN, MX, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SE, SG, SK, TJ, TM, TN, TR, TT, UA, US, UZ, VC, VN, YU, ZA, ZW
RW: AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR

PRIORITY APPLN. INFO.: GB 2002-12413 A 20020529
GB 2003-5684 A 20030312
GB 2003-9219 A 20030423

OTHER SOURCE(S): MARPAT 140:16736

GI



I

AB The invention relates to the use of diaryl urea derivs. [I; G is not present and Z = a radical of the formula Q; A = CH, N, N→O; A1 = N, N→O, with the proviso that not more than one of A and A1 can be N→O; n = 1, 2; m = 0-2; p = 0, 2, 3; q = 0-5; X = (un)substituted NH if p = 0; or if p is 2 or 3, X = nitrogen which together with (CH2)p and the bonds represented in dotted (interrupted) lines (including the atoms to which they are bound) forms a ring, or X = CHK (wherein K = H or lower alkyl) and p = 0, with the proviso that the bonds represented in dotted lines, if p = 0, are absent; Y1 = O, S, CH2; Y2 = O, S, NH; with the proviso that (Y1)n-(Y2)m does not include O-O, S-S, NH-O, NH-S or S-O groups; R1, R2, R3, R5 = independently H or an inorg. or organic moiety or any two of them together form a lower alkylenedioxy bridge bound via the oxygen atoms, and the remaining one of these moieties is hydrogen or an inorg. or organic moiety; R4 (if present, i.e., if q is not zero) is an inorg. or organic moiety] or tautomers thereof or pharmaceutically acceptable salts thereof in the treatment of protein kinase dependent diseases or for the manufacture of pharmaceutical compns. for use in the treatment of said diseases, especially a proliferative disease depending on any one or more of the

following (tyrosine) protein kinases such as ras, Abl, VEGF-receptor tyrosine kinase, Flt3, and/or Bcr-Abl activity. Also disclosed are the use of the compds. I for the manufacture of pharmaceutical compns. for use in the treatment of said diseases, methods of use of the compds. I in the treatment of said diseases, pharmaceutical prepns. comprising the compds. I for the treatment of said diseases, processes for the manufacture of the compds. I, the use or methods of use of the compds. I as mentioned above, and/or the compds. I for use in the treatment of the animal or human body. For example, N-(4-(pyridin-4-yloxy)phenyl)-N'-(4-2,2,2-trifluoroethoxy-3-trifluoromethylphenyl)urea and N-[4-[6-(4-hydroxyphenylamino)pyrimidin-4-yl]phenyl]-N'-(4-2,2,2-trifluoroethoxy-3-trifluoromethylphenyl)urea at 10 μM inhibited gene c-Abl protein kinase by 98%, Kdr receptor tyrosine kinase by 100 and 96%, resp., and Flt3 receptor tyrosine kinase by 100%.

IC ICM C07C275-00

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 7, 27, 63

IT **393-15-7P**, 4-Methoxy-3-trifluoromethylphenylamine 2802-62-2P, 4,6-Difluoropyrimidine 15862-01-8P, 2-Methoxy-4-nitrobiphenyl 20566-90-9P, 3-Nitro-N,N-dimethyl-5-trifluoromethylbenzamide 22227-42-5P, (Piperidin-1-yl)(3-nitro-5-trifluoromethylphenyl)methanone 56970-24-2P, 2-Methoxybiphenyl-4-ylamine 58609-19-1P 70339-06-9P, 4-Piperidin-1-yl-3-trifluoromethylphenylamine 102877-78-1P,

4-(Pyridin-4-yloxy)phenylamine 105130-28-7P, 4-(6-Chloropyrimidin-4-yloxy)aniline 105296-03-5P 105298-89-3P 105350-42-3P 118450-89-8P, 1-(2-Methoxy-4-nitrophenyl)piperidine 124041-03-8P, 4-Chloro-6-(4-nitrophenoxy)pyrimidine 168050-39-3P, (4-Aminobenzyl)carbamic acid benzyl ester 186090-34-6P 252918-98-2P 260783-12-8P, (4-Chloropyridin-2-yl)pyrrolidin-1-ylmethanone 330796-48-0P, 4-(4-Methylpiperazin-1-yl)-3-trifluoromethylphenylamine 417724-25-5P, 6-(4-Aminophenoxy)pyrimidin-4-ylamine 630125-30-3P, Methyl[4-(pyridin-4-yloxy)phenyl]amine 630125-32-5P, N-(4-Ethylphenyl)-2-(4-hydroxyphenyl)acetamide 630125-33-6P 630125-34-7P, 5-(Pyridin-4-yloxy)-2,3-dihydroindole 630125-35-8P, 6-(Pyridin-4-yloxy)-1,2,3,4-tetrahydroquinoline 630125-36-9P, 6-(Pyridin-4-yloxy)quinoline 630125-37-0P 630125-38-1P, [6-(4-Aminophenoxy)pyrimidin-4-yl][4-(tert-butyldimethylsilyloxy)phenyl]amine 630125-39-2P, [4-(tert-Butyldimethylsilyloxy)phenyl][6-(4-nitrophenoxy)pyrimidin-4-yl]amine 630125-40-5P, 4-[6-(4-Nitrophenoxy)pyrimidin-4-ylamino]phenol 630125-41-6P, 3-Chloro-4-(pyridin-4-yloxy)phenylamine 630125-43-8P, [6-(4-Aminophenoxy)pyrimidin-4-yl](4-methoxyphenyl)amine 630125-44-9P, (4-Methoxyphenyl)[6-(4-nitrophenoxy)pyrimidin-4-yl]amine 630125-45-0P 630125-46-1P 630125-47-2P 630125-48-3P 630125-50-7P 630125-51-8P, [4-(Benzyloxycarbonylaminomethyl)phenyl]carbamic acid tert-butyl ester 630125-52-9P, 4-(4-Ethylpiperazin-1-yl)-3-methoxyphenylamine 630125-53-0P, 1-Ethyl-4-(2-methoxy-4-nitrophenyl)piperazine 630125-54-1P, 3-Methoxy-4-(piperidin-1-ylmethyl)phenylamine 630125-55-2P, 1-(2-Methoxy-4-nitrobenzyl)piperidine 630125-56-3P, (2-Methoxy-4-nitrophenyl)piperidin-1-ylmethanone 630125-57-4P, 4-(4-Ethylaminopyrimidin-6-yloxy)aniline 630125-58-5P, 4-(4-Aminophenoxy)-2-methoxypyridine 630125-59-6P, 2-Methoxy-4-(4-nitrophenoxy)pyridine 630125-60-9P, 1-Methyl-4-(4-nitrophenoxy)-1H-pyridin-2-one 630125-61-0P, 4-(4-Nitrophenoxy)-1H-pyridin-2-one 630125-62-1P, 3-(4-Aminophenoxy)-1H-pyridin-6-one 630125-63-2P, 3-(4-Nitrophenoxy)-1H-pyridin-6-one 630125-64-3P, 4-(6-Methoxypyridin-3-ylmethyl)phenylamine 630125-65-4P 630125-66-5P 630125-67-6P, [4-(4-Aminophenoxy)pyridin-2-yl]pyrrolidin-1-ylmethanone 630125-68-7P 630125-69-8P, 4-(4-Aminophenoxy)pyridine-2-carbonitrile 630125-70-1P, 4-(2-Chloropyridin-4-yloxy)phenylamine 630125-71-2P, 4-(2-Trifluoromethylpyridin-4-yloxy)phenylamine 630125-72-3P, 4-(4-Nitrophenoxy)-2-trifluoromethylpyridine 630125-73-4P, 4-(6-Fluoropyrimidin-4-yloxy)phenylamine 630125-74-5P, 4-(6-Trifluoromethylpyrimidin-4-yloxy)phenylamine 630125-75-6P, [4-(6-Chloropyrimidin-4-ylmethyl)phenyl]carbamic acid tert-butyl ester 630125-76-7P, 4-(6-Chloropyrimidin-4-ylmethyl)phenylamine 630125-77-8P, [4-(6-Hydroxypyrimidin-4-ylmethyl)phenyl]carbamic acid tert-butyl ester 630125-78-9P, [4-(6-Hydroxy-2-mercaptopyrimidin-4-ylmethyl)phenyl]carbamic acid tert-butyl ester 630125-79-0P 630125-80-3P, [6-(4-Aminobenzyl)pyrimidin-4-yl]methylamine 630125-81-4P, 4-[2-(1H-Tetrazol-5-yl)pyridin-4-yloxy]phenylamine 630125-82-5P, 3-Trifluoromethyl-4-(piperidin-1-ylmethyl)phenylamine 630125-83-6P, 2,2,2-Trifluoro-N-(4-piperidin-1-ylmethyl-3-trifluoromethylphenyl)acetamide 630125-84-7P 630125-85-8P 630125-86-9P, 3-Methoxy-4-(4-methylpiperazin-1-ylmethyl)phenylamine 630125-87-0P, 3-Methoxy-4-(4-methylpiperazin-1-ylmethyl)nitrobenzene 630125-88-1P, (4-Methylpiperazin-1-yl)(4-nitro-2-methoxyphenyl)methanone 630125-89-2P, 3-Trifluoromethyl-5-(piperidin-1-ylmethyl)phenylamine 630125-90-5P 630125-91-6P, 3-Trifluoromethyl-4-(4-ethylpiperazin-1-ylmethyl)phenylamine 630125-92-7P 630125-93-8P, 3-(4-Ethylpiperazin-1-ylmethyl)-5-trifluoromethylphenylamine 630125-94-9P, (3-Amino-5-trifluoromethylphenyl)(4-ethylpiperazin-1-yl)methanone 630125-95-0P, (3-Nitro-5-trifluoromethylphenyl)(4-ethylpiperazin-1-yl)methanone

630125-96-1P, 4-Chloro-6-(4-isocyanatophenoxy)pyrimidine 630125-97-2P
630125-98-3P, 3-Amino-N,N-dimethyl-5-trifluoromethylbenzamide
630125-99-4P, [6-(4-Aminophenoxy)pyrimidin-4-yl]methylamine
630126-00-0P, 3-Pyridin-2-yl-5-trifluoromethylphenylamine 630126-01-1P,
Methyl[4-(4-nitrophenoxy)pyrimidin-2-yl]amine 630126-02-2P,
2-Chloro-4-(4-nitrophenoxy)pyrimidine 630126-03-3P, 4-(2-Methylimidazol-
1-yl)-3-trifluoromethylphenylamine 630126-05-5P, 2-Methyl-1-(4-nitro-2-
trifluoromethylphenyl)-1H-imidazole 630126-07-7P, [6-(4-Amino-2-
methylphenoxy)pyrimidin-4-yl]methylamine 630126-09-9P,
[3-Methyl-4-(6-methylaminopyrimidin-4-yloxy)phenyl]carbamic acid benzyl
ester 630126-11-3P, [4-(6-Chloropyrimidin-4-yloxy)-3-
methylphenyl]carbamic acid benzyl ester 630126-12-4P,
(4-Hydroxy-3-methylphenyl)carbamic acid benzyl ester 630126-13-5P,
6-(4-Aminobenzyl)pyrimidin-4-ylamine 630126-14-6P, [4-(6-Aminopyrimidin-
4-ylmethyl)phenyl]carbamic acid tert-butyl ester 630126-15-7P,
[4-(6-Azidopyrimidin-4-ylmethyl)phenyl]carbamic acid tert-butyl ester
630126-16-8P, 5-(6-Chloropyrimidin-4-yloxy)-1H-indole 630126-17-9P,
5-(6-Chloropyrimidin-4-yloxy)-2,3-dihydro-1H-indole
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(intermediate; preparation of diarylurea derivs. useful for the treatment of
protein kinase dependent diseases and proliferative diseases)

IT 228400-22-4P 228400-61-1P 228400-77-9P 630122-37-1P 630122-38-2P
630122-39-3P 630122-40-6P 630122-41-7P 630122-42-8P 630122-43-9P
630122-44-0P 630122-46-2P 630122-48-4P 630122-50-8P
630122-51-9P 630122-52-0P 630122-53-1P 630122-54-2P 630122-55-3P
630122-56-4P 630122-57-5P 630122-58-6P 630122-59-7P 630122-60-0P
630122-61-1P 630122-62-2P 630122-63-3P 630122-64-4P 630122-65-5P
630122-66-6P 630122-67-7P **630122-68-8P** 630122-69-9P
630122-70-2P 630122-71-3P, N-[4-(Pyridin-4-yloxy)-3-chlorophenyl]-N'-(3-
trifluoromethylphenyl)urea 630122-72-4P, N-[4-(Pyridin-4-yloxy)-3-
methylphenyl]-N'-(3-trifluoromethylphenyl)urea 630122-73-5P
630122-74-6P 630122-75-7P 630122-76-8P 630122-77-9P 630122-78-0P
630122-79-1P **630122-80-4P**, 5-(Pyridin-4-yloxy)-2,3-dihydroindole-
1-carboxylic acid [4-(2,2,2-trifluoroethoxy)-3-trifluoromethylphenyl]amide
630122-81-5P 630122-82-6P 630122-83-7P 630122-84-8P 630122-85-9P
630122-86-0P 630122-87-1P 630122-88-2P 630122-89-3P 630122-90-6P
630122-91-7P 630122-92-8P 630122-93-9P 630122-94-0P 630122-95-1P
630122-96-2P 630122-97-3P 630122-98-4P 630122-99-5P 630123-00-1P
630123-01-2P 630123-02-3P 630123-03-4P 630123-04-5P 630123-05-6P
630123-06-7P 630123-07-8P 630123-08-9P 630123-09-0P 630123-10-3P
630123-11-4P 630123-12-5P 630123-14-7P, N-[4-(6-Chloropyrimidin-4-
yloxy)phenyl]-N'-(4-tert-butylphenyl)urea 630123-15-8P,
N-[4-(6-Chloropyrimidin-4-yloxy)phenyl]-N'-(4-chloro-3-
trifluoromethylphenyl)urea 630123-16-9P, N-[4-(4-Methylaminopyrimidin-6-
yloxy)phenyl]-N'-(4-tert-butylphenyl)urea 630123-18-1P,
N-[4-(4-Benzylaminopyrimidin-6-yloxy)phenyl]-N'-(4-tert-butylphenyl)urea
630123-20-5P, N-[4-(4-Aminopyrimidin-6-yloxy)phenyl]-N'-(4-chloro-3-
trifluoromethylphenyl)urea 630123-22-7P 630123-24-9P,
N-[4-(6-Chloropyrimidin-4-yloxy)phenyl]-N'-[4-(4-ethylpiperazin-1-yl)-3-
methoxyphenyl]urea 630123-26-1P, N-[4-(4-Chloropyrimidin-6-yloxy)phenyl]-
N'-[3-methoxy-4-(piperidin-1-ylmethyl)phenyl]urea 630123-28-3P
630123-30-7P 630123-32-9P 630123-34-1P 630123-36-3P 630123-38-5P
630123-40-9P 630123-41-0P 630123-43-2P 630123-45-4P 630123-47-6P
630123-49-8P 630123-51-2P 630123-53-4P 630123-55-6P 630123-56-7P
630123-57-8P 630123-59-0P 630123-61-4P 630123-63-6P 630123-65-8P
630123-67-0P 630123-69-2P 630123-70-5P 630123-71-6P 630123-72-7P
630123-73-8P 630123-74-9P 630123-75-0P 630123-76-1P 630123-77-2P
630123-78-3P 630123-79-4P 630123-80-7P 630123-81-8P 630123-82-9P

630123-83-0P 630123-84-1P 630123-85-2P 630123-86-3P 630123-87-4P
630123-89-6P, N-[4-(6-Oxo-1,6-dihydropyridin-3-ylmethyl)phenyl]-N'-(4-methylphenyl)urea 630123-91-0P 630123-92-1P 630123-93-2P
630123-94-3P 630123-95-4P 630123-96-5P 630123-97-6P 630123-98-7P
630123-99-8P 630124-00-4P 630124-01-5P 630124-02-6P 630124-03-7P
630124-04-8P 630124-05-9P 630124-06-0P 630124-07-1P 630124-08-2P
630124-09-3P 630124-10-6P 630124-11-7P 630124-12-8P 630124-13-9P
630124-14-0P 630124-15-1P 630124-16-2P 630124-17-3P 630124-18-4P
630124-19-5P 630124-20-8P 630124-21-9P 630124-22-0P 630124-23-1P
630124-24-2P 630124-25-3P 630124-26-4P, N-[4-(4-Chloropyrimidin-6-yloxy)phenyl]-N'-[3-trifluoromethyl-4-(piperidin-1-ylmethyl)phenyl]urea
630124-27-5P, N-[4-(4-Chloropyrimidin-6-yloxy)phenyl]-N'-[3-methoxy-4-(4-methylpiperazin-1-ylmethyl)phenyl]urea 630124-28-6P,
N-[4-(4-Azidopyrimidin-6-yloxy)phenyl]-N'-[3-trifluoromethyl-4-(piperidin-1-ylmethyl)phenyl]urea 630124-29-7P 630124-30-0P, N-[4-(4-Chloropyrimidin-6-yloxy)phenyl]-N'-[3-trifluoromethyl-5-(piperidin-1-ylmethyl)phenyl]urea 630124-32-2P, N-[4-(4-Chloropyrimidin-6-yloxy)phenyl]-N'-[3-trifluoromethyl-4-(4-ethylpiperazin-1-ylmethyl)phenyl]urea 630124-34-4P, N-[4-(6-Chloropyrimidin-4-yloxy)phenyl]-N'-[5-trifluoromethyl-3-[(4-ethylpiperazin-1-yl)methyl]phenyl]urea 630124-36-6P, N-[4-(6-Chloropyrimidin-4-yloxy)phenyl]-N'-[5-trifluoromethyl-3-(dimethylaminomethyl)phenyl]urea
630124-37-7P 630124-38-8P 630124-39-9P 630124-40-2P 630124-42-4P
630124-44-6P 630124-46-8P 630124-48-0P 630124-50-4P 630124-52-6P
630124-53-7P 630124-54-8P 630124-55-9P 630124-56-0P 630124-57-1P
630124-58-2P 630124-59-3P 630124-60-6P 630124-61-7P 630124-62-8P
630124-63-9P 630124-64-0P 630124-65-1P 630124-66-2P 630124-67-3P
630124-68-4P 630124-69-5P 630124-70-8P 630124-71-9P 630124-72-0P
630124-73-1P 630124-74-2P 630124-75-3P 630124-77-5P 630124-78-6P
630124-80-0P 630124-81-1P 630124-82-2P 630124-84-4P
630124-86-6P 630124-88-8P 630124-90-2P 630124-92-4P 630124-94-6P
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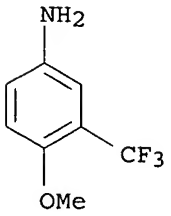
630125-16-5P 630125-20-1P 630125-22-3P 630125-24-5P 630125-26-7P
630125-27-8P 630125-28-9P 630125-29-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of diarylurea derivs. useful for the treatment of protein kinase dependent diseases and proliferative diseases)

IT 60-35-5, Acetamide, reactions 62-56-6, Thiourea, reactions 74-88-4, Methyl iodide, reactions 74-89-5, Methylamine, reactions 75-04-7, Ethylamine, reactions 75-44-5, Phosgene 98-16-8, 3-Trifluoromethylphenylamine 98-80-6, Phenylboronic acid 100-00-5, 1-Chloro-4-nitrobenzene 100-02-7, 4-Nitrophenol, reactions 100-46-9, Benzylamine, reactions 104-94-9, p-Anisidine 109-01-3, 1-Methylpiperazine 110-89-4, Piperidine, reactions 111-95-5 123-30-8, 4-Aminophenol 123-75-1, Pyrrolidine, reactions 156-38-7, 4-Hydroxyphenylacetic acid 327-78-6, 4-Chloro-3-trifluoromethylphenyl isocyanate 328-80-3 329-01-1, 3-(Trifluoromethyl)phenyl isocyanate 350-46-9, 4-Fluoronitrobenzene 367-67-9, 1-Bromo-4-nitro-2-trifluoromethylbenzene 407-25-0, Trifluoroacetic acid anhydride 501-53-1, Chloroformic acid benzyl ester 506-59-2, Dimethylamine hydrochloride 555-16-8, 4-Nitrobenzaldehyde, reactions 586-95-8, 4-Hydroxymethylpyridine 589-16-2, 4-Ethylaniline 591-27-5, 3-Aminophenol 622-58-2, 4-Methylphenyl isocyanate 626-03-9, 2,4-Dihydroxypyridine 626-61-9, 4-Chloropyridine **654-76-2**, 1-Methoxy-4-nitro-2-trifluoromethylbenzene 693-98-1, 2-Methylimidazole 917-54-4, Methyllithium 1124-33-0, 4-Nitropyridine N-oxide 1193-21-1, 4,6-Dichloropyrimidine 1943-67-5, 4-tert-Butylphenyl isocyanate

1953-54-4, 5-Hydroxyindole 2597-56-0, 2-Methoxy-4-nitrobenzoic acid 2835-96-3, 4-Amino-2-methylphenol 3934-20-1, 2,4-Dichloropyrimidine 5154-01-8, 2,5-Dihydroxypyridine 5308-25-8, N-Ethylpiperazin 7379-35-3, 4-Chloropyridine hydrochloride 7677-24-9, Trimethylsilyl cyanide 7789-23-3, Potassium fluoride 13472-85-0, 5-Bromo-2-methoxypyridine 17997-47-6, 2-Tributylstannylpyridine 18162-48-6, tert-Butyldimethylsilyl chloride 23056-36-2, 2-Chloro-4-nitropyridine 23138-50-3 24424-99-5, Di-tert-butyl dicarbonate 24484-93-3, 4-Chloropyridine-2-carboxylic acid methyl ester 26628-22-8, Sodium azide 27692-74-6, 4-(Pyridin-4-ylmethyl)phenylamine 32315-10-9, Triphosgene 35019-96-6, trans-2-Phenylcyclopropyl isocyanate 37552-81-1, 4-Chloro-6-trifluoromethylpyrimidine 54962-75-3, 3-Amino-5-bromobenzotrifluoride 62088-12-4 65934-74-9, 5-Amino-2-methylbenzotrifluoride 77337-82-7, 1-Bromo-2-methoxy-4-nitrobenzene 105316-06-1, 4-Morpholin-4-yl-3-trifluoromethylphenylamine 109903-35-7 170886-13-2, 2-Trifluoromethylpyridin-4-ol 220298-96-4, 4-(Aminomethyl)-N-(tert-butoxycarbonyl)aniline 321352-53-8, (R)-5-Bromoindan-2-ylamine 417724-26-6, 4-(4-Aminophenoxy)pyrimidin-2-ylamine 630123-88-5, N-[4-(6-Methoxypyridin-3-ylmethyl)phenyl]-N'-(4-methylphenyl)urea 630123-90-9 630125-31-4, Methyl[4-(pyridin-4-ylmethyl)phenyl]amine 630125-42-7 630125-49-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; preparation of diarylurea derivs. useful for the treatment of protein kinase dependent diseases and proliferative diseases)

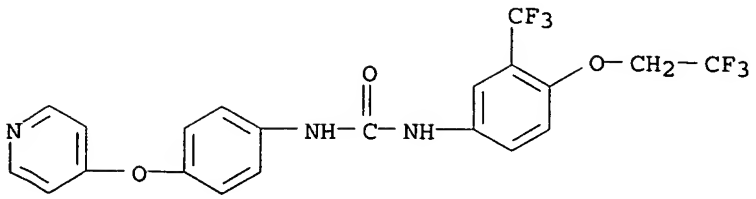
IT **393-15-7P**, 4-Methoxy-3-trifluoromethylphenylamine
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of diarylurea derivs. useful for the treatment of protein kinase dependent diseases and proliferative diseases)

RN 393-15-7 HCAPLUS
CN Benzenamine, 4-methoxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

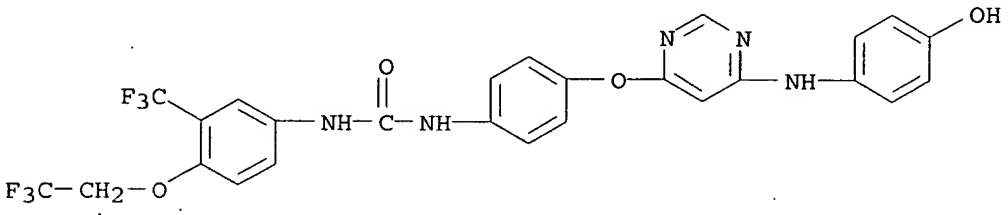


IT **630122-44-0P 630122-68-8P 630122-80-4P**,
5-(Pyridin-4-yloxy)-2,3-dihydroindole-1-carboxylic acid [4-(2,2,2-trifluoroethoxy)-3-trifluoromethylphenyl]amide
630124-80-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of diarylurea derivs. useful for the treatment of protein kinase dependent diseases and proliferative diseases)

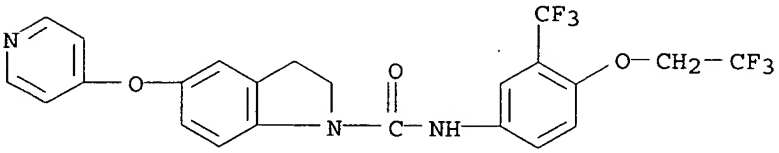
RN 630122-44-0 HCAPLUS
CN Urea, N-[4-(4-pyridinyloxy)phenyl]-N'-[4-(2,2,2-trifluoroethoxy)-3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 630122-68-8 HCAPLUS
CN Urea, N-[4-[[6-[(4-hydroxyphenyl)amino]-4-pyrimidinyl]oxy]phenyl]-N'-[4-(2,2,2-trifluoroethoxy)-3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 630122-80-4 HCAPLUS
CN 1H-Indole-1-carboxamide, 2,3-dihydro-5-(4-pyridinyloxy)-N-[4-(2,2,2-trifluoroethoxy)-3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 630124-80-0 HCAPLUS
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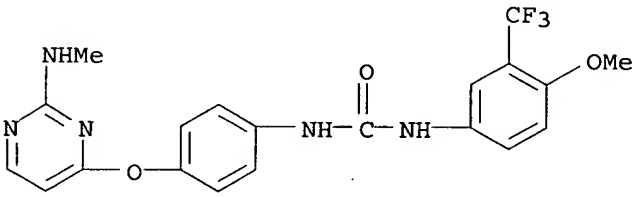
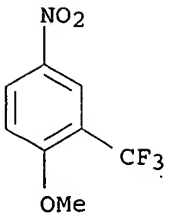
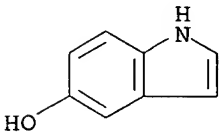


IT **654-76-2**, 1-Methoxy-4-nitro-2-trifluoromethylbenzene
1953-54-4, 5-Hydroxyindole
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; preparation of diarylurea derivs. useful for the treatment of protein kinase dependent diseases and proliferative diseases)
RN 654-76-2 HCAPLUS
CN Benzene, 1-methoxy-4-nitro-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)



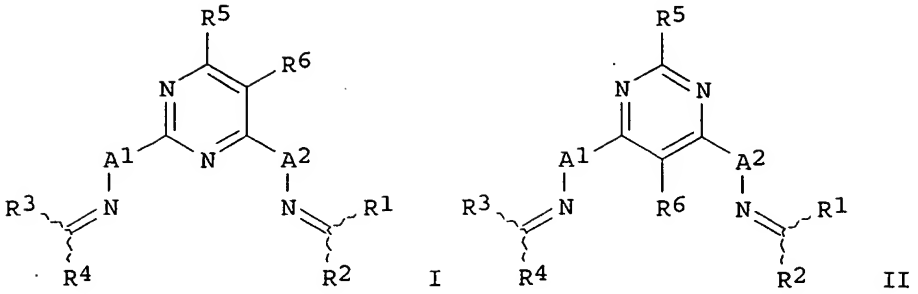
RN 1953-54-4 HCAPLUS
CN 1H-Indol-5-ol (9CI) (CA INDEX NAME)



L33 ANSWER 3 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:875259 HCAPLUS
DOCUMENT NUMBER: 139:364950
TITLE: Preparation of pyrimidine derivatives as mixed lymphocyte reaction (MLR) inhibitors
INVENTOR(S): Tsuruoka, Hiroyuki; Kanno, Yuichi; Tatsuta, Tohru
PATENT ASSIGNEE(S): Sankyo Company, Limited, Japan
SOURCE: PCT Int. Appl., 420 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003091223	A1	20031106	WO 2003-JP5216	20030423
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2004002391	A2	20040108	JP 2003-113563	20030418
PRIORITY APPLN. INFO.:			JP 2002-120608 A	20020423
OTHER SOURCE(S):	MARPAT 139:364950			

GI



I II

AB Pyrimidines derivs. such as dihydrazinopyrimidine having the general formula (I) and (II) [wherein R1, R3 = H, lower alkyl, halo-lower alkyl, lower alkoxy-lower alkyl, mono- or di(lower alkyl)amino-lower alkyl, (un)substituted aryl; R2, R4 = each (un)substituted aryl or heterocyclyl; or CR2R1 or CR4R3 together forms an (un)substituted saturated carbocyclic or heterocyclic ring; A1, A2 = NR7, O (wherein R7 = lower alkyl); R5 lower alkylthio, each (un)substituted cycloalkyl, aryl, or heterocyclyl, a group having the formula -D-R8 or CH2-E-R8 (wherein D = NH, O, S; E = O, S, a single bond; R8 = each optionally substituted cycloalkyl, aryl, or heterocyclyl, etc.); R6 = H, lower alkyl, lower alkoxy, lower alkoxy-lower alkyl, mono- or di(lower alkyl)amino-lower alkyl, aralkyl, anilino], pharmaceutically acceptable salts, esters, or other derivs. thereof. are prepared These pyrimidine derivs. exhibit excellent MLR inhibiting action and are useful for inhibiting allograft rejection in bone marrow or organ transplant or for the treatment and/or prevention of inflammation, organ-specific or organ-nonspecific autoimmune diseases, or allergy, in particular chronic articular rheumatism, multiple sclerosis, inflammatory enteric disease, diabetes, glomerulonephritis, idiopathic biliary cirrhosis, active chronic hepatitis, pernicious anemia, Hashimoto thyroiditis, atrophic gastritis, myasthenia gravis, psoriasis, Sjoegren's syndrome, systemic lupus erythematosus, rhinitis, asthma, or atopic dermatitis. They are also useful for inhibiting cancer cells, in particular cancerous lymphocyte. Thus, 480 mg N-(2,6-dichloropyrimidin-4-yl)phenylamine was stirred with 3 mL hydrazine monohydrate at 90° for 1 h, cooled to room temperature, treated with H2O, followed by filtering the precipitated crystals, washing them with water, Et acetate, and drying under reduced pressure to give crude N-(2,6-dihydrazinopyrimidin-4-yl)phenylamine. The latter compound was dissolved in 5 mL dioxane, treated with 1.7 mL 4-acetylpyridine, refluxed for 15 h, distilled to remove the solvent, and suspended in a mixture of ether and Et acetate, followed by pulverizing the precipitated solid, filtration, and washing with a mixture of ether and Et acetate to give 1-(4-pyridinyl)-1-ethanone N-[4-anilino-6-[2-[1-(4-pyridinyl)ethylidene]hydrazino]-2-pyrimidinyl]hydrazone (III). In an MLR inhibition assay, III and 1-(4-pyridinyl)-1-ethanone N-[2-anilino-6-[2-[1-(4-pyridinyl)ethylidene]hydrazino]-4-pyrimidinyl]hydrazone in vitro inhibited the uptake of [3H]thymidine in human peripheral lymphocyte with IC50 of 6.9 and 1.0 nM, resp.

IC ICM C07D239-50
ICS C07D401-14; C07D403-14; C07D409-14; C07D417-14; A61K031-505; A61K031-506; A61P001-00; A61P001-04; A61P001-16; A61P003-10; A61P007-06; A61P011-02; A61P011-06; A61P013-12; A61P017-00; A61P017-06; A61P019-02; A61P021-04; A61P025-00

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

IT 620979-82-0P 620979-83-1P 620979-84-2P 620979-85-3P 620979-86-4P
620979-87-5P 620979-88-6P 620979-89-7P 620979-90-0P 620979-91-1P
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620980-02-1P 620980-03-2P 620980-04-3P 620980-05-4P 620980-06-5P
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620982-18-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidine derivs. as mixed lymphocyte reaction inhibitors for treatment of cancer or allograft rejection and for treatment and/or prevention of inflammation, organ-(non)specific autoimmune diseases, or allergy)

IT 62-53-3, Aniline, reactions 64-04-0, 2-Phenylethylamine 83-13-6, Diethyl phenylmalonate 87-59-2, 2,3-Dimethylaniline 90-04-0, 2-Methoxyaniline 90-05-1, 2-Methoxyphenol 94-09-7, Ethyl 4-aminobenzoate 95-51-2, 2-Chloroaniline 95-64-7, 3,4-Dimethylaniline

95-68-1, 2,4-Dimethylaniline **95-69-2**, 2-Methyl-4-chloroaniline
95-76-1, 3,4-Dichloroaniline 97-50-7 98-16-8, 3-Trifluoromethylaniline
99-09-2, 3-Nitroaniline 99-88-7, 4-Isopropylaniline 99-98-9,
4-Dimethylaminoaniline 100-01-6, 4-Nitroaniline, reactions 100-61-8,
N-Methylaniline, reactions 102-50-1, 2-Methyl-4-methoxyaniline
104-13-2, 4-n-Butylaniline 104-94-9, 4-Methoxyaniline 104-96-1,
4-Methylthioaniline 105-53-3, Diethyl malonate 106-40-1,
4-Bromoaniline 106-47-8, 4-Chloroaniline, reactions 106-49-0,
4-Methylaniline, reactions 108-42-9, 3-Chloroaniline 108-44-1,
3-Methylaniline, reactions 108-69-0, 3,5-Dimethylaniline 108-91-8,
Cyclohexylamine, reactions 110-89-4, Piperidine, reactions 121-90-4,
3-Nitrobenzoyl chloride 122-04-3, 4-Nitrobenzoyl chloride 123-08-0,
4-Hydroxybenzaldehyde 123-75-1, Pyrrolidine, reactions 124-63-0,
Methanesulfonyl chloride 133-13-1, Diethyl ethylmalonate 139-59-3,
4-Phenoxyaniline 142-04-1, Aniline hydrochloride 153-78-6,
2-Aminofluorene 156-43-4, 4-Ethoxyaniline 321-73-3 348-54-9,
2-Fluoroaniline 366-99-4, 3-Fluoro-4-methoxyaniline 367-21-5,
3-Chloro-4-fluoroaniline 367-25-9, 2,4-Difluoroaniline 367-29-3,
2-Methyl-5-fluoroaniline 367-30-6, 2,5-Difluoroaniline 367-34-0,
2,4,5-Trifluoroaniline 369-68-6, 3-Trifluoromethylthioaniline
371-40-4, 4-Fluoroaniline 372-19-0, 3-Fluoroaniline 372-39-4,
3,5-Difluoroaniline 420-04-2, Cyanamide 437-83-2 443-86-7,
2-Methyl-3-fluoroaniline 452-69-7 452-71-1, 2-Methyl-4-fluoroaniline
452-77-7, 3-Fluoro-4-methylaniline 452-84-6, 2-Fluoro-5-methylaniline
455-14-1, 4-Trifluoromethylaniline 458-52-6, 2-Fluoro-4-methoxyaniline
461-82-5, 4-Trifluoromethoxyaniline 462-08-8, 3-Aminopyridine
496-15-1, Indoline 536-90-3, 3-Methoxyaniline 578-54-1, 2-Ethylaniline
580-15-4, 6-Aminoquinoline 589-16-2, 4-Ethylaniline 591-19-5,
3-Bromoaniline 607-81-8, Diethyl benzylmalonate 609-08-5, Diethyl
methylmalonate 621-33-0, 3-Ethoxyaniline 626-43-7, 3,5-Dichloroaniline
636-21-5, 2-Methylaniline hydrochloride 656-65-5 685-87-0, Diethyl
bromomalonate 704-13-2, 3-Hydroxy-4-nitrobenzaldehyde 713-67-7
831-75-4, 3-(1,1,2,2-Tetrafluoroethoxy)aniline 1072-82-8,
3-Acetylpyrrole 1122-54-9, 4-Acetylpyridine 1135-12-2, 4-Benzylaniline
1535-73-5, 3-Trifluoromethoxyaniline 1544-85-0, 2,2-
Difluorobenzo[1,3]dioxol-5-ylamine 1670-14-0 1783-81-9,
3-Methylthioaniline 1788-10-9, 4-Acetylbenzenesulfonyl chloride
2106-04-9, 2-Fluoro-3-chloroaniline 2106-05-0 2163-48-6, Diethyl
propylmalonate 2243-47-2, 3-Biphenylamine 2357-47-3,
3-Trifluoromethyl-4-fluoroaniline 2380-36-1, 3,5-Di-tert-butylaniline
2696-84-6, 4-n-Propylaniline 2987-53-3, 2-Methylthioaniline 3586-12-7,
3-Phenoxyaniline 3764-01-0, 2,4,6-Trichloropyrimidine 3863-11-4,
3,4-Difluoroaniline 4023-02-3 4518-10-9, Methyl 3-aminobenzoate
4519-40-8, 2,3-Difluoroaniline 4534-10-5, 3-Methyl-4-isopropylaniline
5018-30-4, Dimethyl methoxymalonate 5369-19-7, 3-tert-Butylaniline
5438-70-0, Ethyl 4-aminophenylacetate 5470-11-1, Hydroxylamine
hydrochloride 5651-14-9, 2-Naphthalenecarboximidamide 6274-18-6
6299-25-8, 2-Methylthio-4,6-dichloropyrimidine 6373-50-8,
4-Cyclohexylaniline 6414-58-0, Diethyl anilinomalonate 6553-96-4,
2,4,6-Triisopropylbenzenesulfonyl chloride 6967-12-0, 1H-Indazol-6-amine
7024-58-0 7664-66-6, 4-Isopropoxyaniline 7803-57-8, Hydrazine
monohydrate 13623-25-1 14268-66-7, Benzo[1,3]dioxol-5-ylamine
16245-79-7, 4-n-Octylaniline 18465-11-7 19335-11-6,
1H-Indazol-5-ylamine 21436-96-4, 2,4-Dimethylaniline hydrochloride
22013-33-8, 2,3-Dihydrobenzo[1,4]dioxin-6-ylamine 22236-08-4,
3-Difluoromethoxyaniline 23255-20-1, Nicotinamidine 24313-88-0,
3,4,5-Trimethoxyaniline 24425-40-9 28840-63-3, 2,4,6-
Trihydrazinopyrimidine 30273-11-1, 4-sec-Butylaniline 33322-60-0,
3-Amino-N,N-dimethylbenzamide 35161-70-7, N-Methylhexylamine

39905-50-5 39905-57-2 40891-33-6, 3,5-Dimethoxyaniline hydrochloride
49742-89-4 50868-72-9, 2-Methyl-5-methoxyaniline 51085-49-5,
2-Fluoroaniline hydrochloride 57946-56-2, 2-Fluoro-4-chloroaniline
64465-53-8, 3-Methoxy-4-fluoroaniline 64628-74-6, 3-Chloro-4-
trifluoromethylthioaniline 67386-38-3, 2-Phenoxyacetamidine
hydrochloride 69411-68-3, 3-Fluoro-4-trifluoromethylaniline 84544-86-5
89808-01-5, 2-Ethoxyaniline hydrochloride 122243-33-8 163733-96-8,
3,4,5-Trifluoroaniline 175136-34-2, 3,4-Dihydro-2H-1,5-benzodioxepin-7-
amine 197147-24-3 207849-43-2 224635-75-0 470702-37-5
500115-27-5 620983-68-8 620983-73-5 620983-88-2 620983-91-7
620983-96-2 620984-69-2 **620984-76-1** 620985-62-8
620985-93-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrimidine derivs. as mixed lymphocyte reaction inhibitors for treatment of cancer or allograft rejection and for treatment and/or prevention of inflammation, organ-(non)specific autoimmune diseases, or allergy)

IT **393-15-7P** 432-86-0P 1565-17-9P, 4-Acetylbenzenesulfonamide
7043-09-6P 13566-71-7P, 2-Phenyl-4,6-dihydroxypyrimidine 14309-78-5P
18303-28-1P 28176-12-7P 28230-47-9P 28230-48-0P 58722-33-1P
60000-87-5P 65399-52-2P 65399-53-3P 68793-19-1P 84755-00-0P
200442-61-1P 204394-77-4P 325685-70-9P 420130-92-3P 500115-23-1P
500115-24-2P 500115-25-3P 500115-29-7P 500115-32-2P 620983-66-6P
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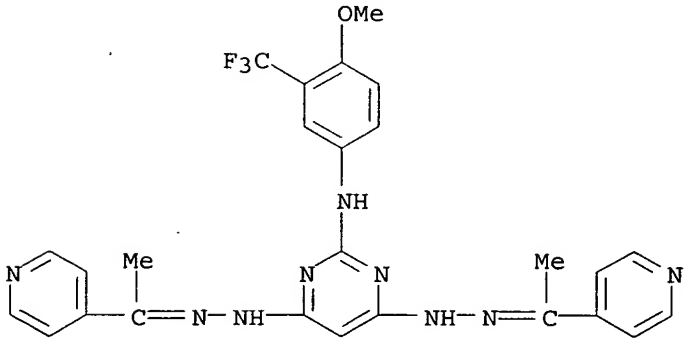
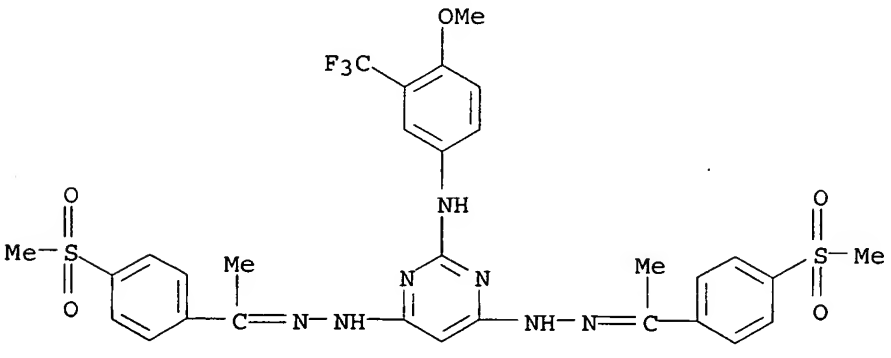
620985-79-7P 620985-80-0P 620985-81-1P 620985-82-2P 620985-83-3P
620985-84-4P 620985-85-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrimidine derivs. as mixed lymphocyte reaction inhibitors for treatment of cancer or allograft rejection and for treatment and/or prevention of inflammation, organ-(non)specific autoimmune diseases, or allergy)

IT **620980-68-9P 620980-71-4P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidine derivs. as mixed lymphocyte reaction inhibitors for treatment of cancer or allograft rejection and for treatment and/or prevention of inflammation, organ-(non)specific autoimmune diseases, or allergy)

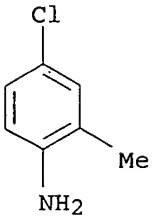
RN 620980-68-9 HCAPLUS
CN 4(1H)-Pyrimidinone, 2-[[4-methoxy-3-(trifluoromethyl)phenyl]amino]-6-[[1-(4-pyridinyl)ethylidene]hydrazino]-, [1-(4-pyridinyl)ethylidene]hydrazone (9CI) (CA INDEX NAME)



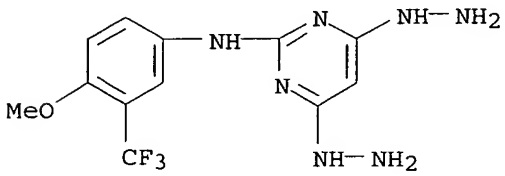
RN 620980-71-4 HCAPLUS
CN 4(1H)-Pyrimidinone, 2-[[4-methoxy-3-(trifluoromethyl)phenyl]amino]-6-[[[4-(methylsulfonyl)phenyl]ethylidene]hydrazino]-, [[4-(methylsulfonyl)phenyl]ethylidene]hydrazone (9CI) (CA INDEX NAME)



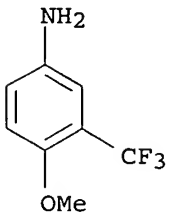
IT **95-69-2**, 2-Methyl-4-chloroaniline **620984-76-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrimidine derivs. as mixed lymphocyte reaction inhibitors for treatment of cancer or allograft rejection and for treatment and/or prevention of inflammation, organ-(non)specific autoimmune diseases, or allergy)
RN 95-69-2 HCAPLUS
CN Benzenamine, 4-chloro-2-methyl- (9CI) (CA INDEX NAME)



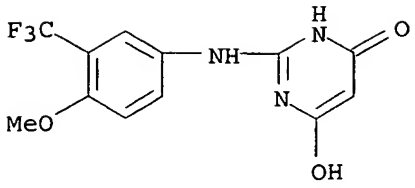
RN 620984-76-1 HCAPLUS
CN 4(1H)-Pyrimidinone, 6-hydrazino-2-[[4-methoxy-3-(trifluoromethyl)phenyl]amino]-, hydrazone (9CI) (CA INDEX NAME)



IT **393-15-7P 620984-75-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrimidine derivs. as mixed lymphocyte reaction inhibitors for treatment of cancer or allograft rejection and for treatment and/or prevention of inflammation, organ-(non)specific autoimmune diseases, or allergy)
RN 393-15-7 HCAPLUS
CN Benzenamine, 4-methoxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 620984-75-0 HCAPLUS
CN 4(1H)-Pyrimidinone, 6-hydroxy-2-[[4-methoxy-3-(trifluoromethyl)phenyl]amino]- (9CI) (CA INDEX NAME)

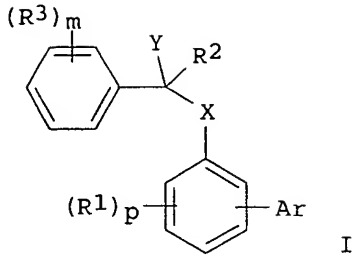


REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

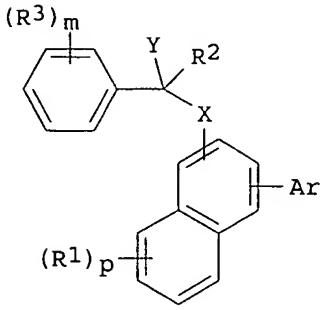
L33 ANSWER 4 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:777734 HCAPLUS
DOCUMENT NUMBER: 139:292242
TITLE: Preparation of heteroarylphenoxyphenylacetates for treating diseases associated with glucose metabolism, lipid metabolism and insulin secretion.
INVENTOR(S): Zhao, Zuchun; Chen, Xin; Wang, Jianchao; Sun, Hongbin; Liang, Jack Shih-Chieh
PATENT ASSIGNEE(S): Metabolex, Inc., USA
SOURCE: PCT Int. Appl., 330 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003080545	A2	20031002	WO 2003-US8899	20030319
WO 2003080545	A3	20040122		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004029933	A1	20040212	US 2003-394487	20030319
PRIORITY APPLN. INFO.:			US 2002-366961P P	20020320

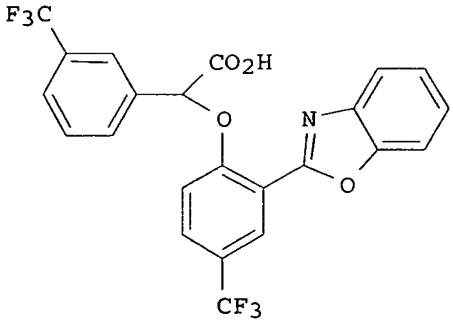
OTHER SOURCE(S): MARPAT 139:292242
GI



I



II



III

AB Title compds. [I, II; X = O, S, SO, SO2, NR; R = H, alkyl, CORa, CO2Ra, CONRaRb; Ra, Rb = H, alkyl; Y = CH2ORc, CO2Rc, CHO, CONRCRm, CH(:NRC), CH(:NORc), carboxylic acid surrogates; Rc = H, alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, aryl, aralkyl, alkylene-Z; Z = CORd, CO2Rd, NRdRe, NRdCONReR, NRdCORe, NRdCO2Re, CONRdRe; Rd, Re, Rf = H, alkyl, Ph; 2 of Rd, Re, Rf attached to the same N form a 5-6 membered ring; Rm = H, alkyl, aryl, OH, SO2Rn; Rn = alkyl, haloalkyl, aralkyl, heteroalkyl, aryl, heteroaryl, alkoxy, aryloxy, (di)alkylamino, (di)arylamino, haloalkylamino, di(haloalkyl)amino; RmRcN = 5-6 membered ring; Ar = (substituted) heteroaryl; q = 0-2; R1, R3 = halo, OH, alkyl, alkenyl, alkynyl, alkoxy, cycloalkyl, cycloalkylalkyl, haloalkyl, heteroalkyl, heterocyclyl, heterosubstituted cycloalkyl, heteroalkyl substituted cycloalkyl, haloalkoxy, NO2, cyano, Ph, PhO, NRj-Ph, SOr-Ph, CORj, CO2Rj, NRJRk, SOrRj, SO2NRjRk, NRJCONRkRi, NRJCORk, NRJCOORk, CONRjRk wherein the Ph ring is optionally substituted and Rj, Rk, Rl = H, alkyl, haloalkyl; 2 of Rj, Rk, Rl when attached to the same N form a 5-6 membered ring; r = 0-2; R2 = H, alkyl, haloalkyl, aralkyl, alkylene-Z; m = 0-4; p = 0-3], were prepared Thus, reaction of 3-F3CC6H4CHBrCO2Et with 2-(2-benzoxazolyl)-4-trifluoromethylphenol followed by saponification with LiOH gave title compound (III). III effectively lowered glucose in mice at ≤25 mg/kg orally.

IC ICM C07C

CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

IT 57-71-6, Diacetyl monoxime 60-34-4, Methylhydrazine 67-63-0, Isopropanol, reactions 71-36-3, 1-Butanol, reactions 78-95-5 88-74-4, 2-Aminonitrobenzene 90-64-2, Phenylhydroxyacetic acid 95-55-6, 2-Aminophenol 95-85-2, 2-Amino-4-chlorophenol 100-63-0, Phenylhydrazine 104-01-8, 4-Methoxyphenylacetic acid 105-36-2, Ethyl bromoacetate 106-48-9, 4-Chlorophenol 108-01-0, 2-(Dimethylamino)ethanol 137-07-5, 2-Aminothiophenol 142-26-7, N-Acetylethanolamine 321-14-2, 2-Hydroxy-5-chlorobenzoic acid

349-10-0, 3-Trifluoromethylmandelic acid 351-35-9, 3-Trifluoromethylphenylacetic acid 402-45-9, 4-Trifluoromethylphenol 455-19-6, 4-Trifluoromethylbenzaldehyde 492-86-4 534-07-6, 1,3-Dichloroacetone 611-71-2 622-40-2, 2-Morpholin-4-ylethanol 624-80-6, Ethylhydrazine 695-96-5, 2-Bromo-4-chlorophenol 696-59-3, 2,5-Dimethoxytetrahydrofuran 835-64-3 917-54-4 1520-70-3, Ethanesulfonamide 1765-93-1 1798-09-0, 3-Methoxyphenylacetic acid 1878-65-5, 3-Chlorophenylacetic acid 1878-66-6, 4-Chlorophenylacetic acid 2075-45-8, 4-Bromopyrazole 2430-01-5, N,N-Diethylbromoacetamide 2440-22-4 2675-89-0, N,N-Dimethyl chloroacetamide 2955-88-6, 2-Pyrrolidin-1-ylethanol 3042-81-7, Methyl 2-bromo-2-phenylacetate 3144-09-0, Methanesulfonamide 3147-75-9 3147-76-0 3315-19-3 3411-95-8 3530-11-8, Butylhydrazine 3966-30-1 4068-78-4, Methyl 2-hydroxy-5-chlorobenzoate 4091-39-8 4595-59-9, 5-Bromopyrimidine 4748-78-1, 4-Ethylbenzaldehyde 5042-30-8, 2,2,2-Trifluoroethylhydrazine 5067-25-4 5292-43-3, tert-Butyl bromoacetate 6329-74-4, 2-Hydroxy-5-bromobenzamide 7120-43-6, 2-Hydroxy-5-chlorobenzamide 7644-04-4, Aminomethyl 4-Bromophenyl ketone 10421-85-9 13113-71-8 14967-45-4 15028-40-7 16273-37-3 **16867-03-1**, 2-Amino-3-hydroxypyridine 17199-29-0 18704-67-1 18997-19-8, Chloromethyl pivalate 22483-09-6, Aminoacetaldehyde dimethyl acetal 23948-77-8, Biphenyl-3-acetic acid 24091-92-7 24243-71-8, 1-Propanesulfonamide 25729-32-2 29684-42-2 32222-43-8 32852-81-6, 3-Phenoxyphenylacetic acid 33533-99-2, 6-Chlorochromone 40299-87-4, N-Bromoacetylmorpholine 51483-92-2, 6-Bromochromone 53731-99-0 54639-55-3 61008-98-8 **77053-56-6** 77053-60-2 77143-76-1 86176-56-9 86215-57-8 90892-09-4, N-Bromoacetylpyrrolidine 91587-47-2 92317-42-5 96464-19-6 115029-23-7, 2-Fluoro-5-trifluoromethylbenzoic acid 132741-29-8 137420-52-1 157033-23-3, 2,5-Difluorophenylacetyl chloride 158548-85-7 163339-67-1 167678-46-8, 3-Acetoxy-2-methylbenzoyl chloride 207981-46-2, 2-Fluoro-5-trifluoromethylbenzoyl chloride 609346-54-5 609352-68-3 609352-69-4 609352-70-7 609352-71-8 609352-72-9 609352-73-0 609352-74-1 609352-75-2 609352-76-3 609352-77-4 609352-78-5 609352-79-6 609352-80-9 609352-81-0 609352-82-1 609352-83-2 609352-84-3 609352-85-4 609352-86-5 609352-87-6 609352-88-7 609352-89-8 609352-90-1 609352-91-2 609352-92-3 609352-93-4 609352-94-5

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of heteroarylphenoxyphenylacetates for treating diseases associated with glucose metabolism, lipid metabolism and insulin secretion)

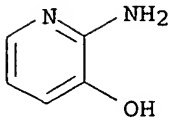
IT 331-33-9P 4184-70-7P 5022-48-0P 5378-21-2P 5445-25-0P 6265-97-0P 33458-32-1P 36124-03-5P 36141-22-7P 36141-23-8P 41023-25-0P 41024-33-3P **50612-99-2P** 51589-62-9P 53732-00-6P 56361-58-1P 59580-38-0P 71229-85-1P 77053-53-3P 156276-22-1P 186026-02-8P 201748-37-0P 202823-24-3P 220532-06-9P 286471-16-7P 303111-34-4P 362007-62-3P 415973-95-4P 609352-24-1P 609352-25-2P 609352-26-3P 609352-27-4P 609352-28-5P 609352-29-6P 609352-30-9P 609352-31-0P 609352-32-1P 609352-33-2P 609352-34-3P 609352-35-4P 609352-36-5P 609352-37-6P 609352-38-7P 609352-39-8P 609352-40-1P 609352-41-2P 609352-42-3P 609352-43-4P 609352-44-5P 609352-45-6P 609352-46-7P 609352-47-8P 609352-48-9P 609352-49-0P 609352-50-3P 609352-51-4P 609352-52-5P 609352-53-6P 609352-54-7P 609352-55-8P 609352-56-9P 609352-57-0P 609352-58-1P 609352-59-2P 609352-60-5P 609352-61-6P 609352-62-7P 609352-63-8P 609352-64-9P 609352-65-0P 609352-66-1P 609352-67-2P 609352-95-6P 609352-96-7P 609352-97-8P 609352-98-9P 609352-99-0P 609353-00-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of heteroarylphenoxyphenylacetates for treating diseases associated with glucose metabolism, lipid metabolism and insulin secretion)

IT **16867-03-1**, 2-Amino-3-hydroxypyridine **77053-56-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of heteroarylphenoxyphenylacetates for treating diseases associated with glucose metabolism, lipid metabolism and insulin secretion)

RN 16867-03-1 HCAPLUS
CN 3-Pyridinol, 2-amino- (6CI, 8CI, 9CI) (CA INDEX NAME)



RN 77053-56-6 HCAPLUS
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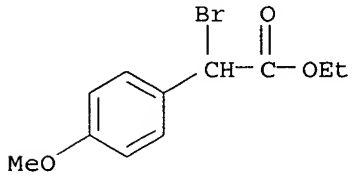
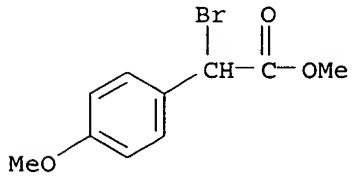


IT **50612-99-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of heteroarylphenoxyphenylacetates for treating diseases associated with glucose metabolism, lipid metabolism and insulin secretion)

RN 50612-99-2 HCAPLUS
CN Benzeneacetic acid, α-bromo-4-methoxy-, methyl ester (9CI) (CA INDEX NAME)



L33 ANSWER 5 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:610204 HCAPLUS
DOCUMENT NUMBER: 139:164801
TITLE: Preparation of 2,4-pyrimidinediamines as IgE and/or IgG receptor modulators for treatment of allergic diseases, inflammatory conditions, and tissue destruction
INVENTOR(S): Singh, Rajinder; Argade, Ankush; Payan, Donald G.; Molineaux, Susan; Holland, Sacha J.; Clough, Jeffrey; Keim, Holger; Bhamidipati, Somasekhar; Sylvain, Catherine; Li, Weigun; Rossi, Alexander B.

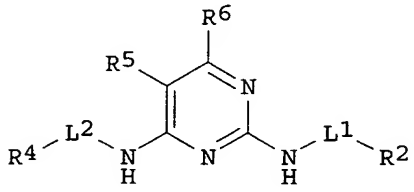
PATENT ASSIGNEE(S): Rigel Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 648 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003063794	A2	20030807	WO 2003-US3022	20030131
WO 2003063794	A3	20031204		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004029902	A1	20040212	US 2003-355543	20030131
EP 1471915	A2	20041103	EP 2003-707654	20030131
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				

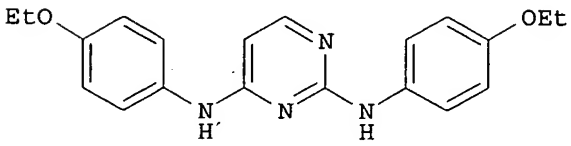
PRIORITY APPLN. INFO.:

US 2002-353267P	P	20020201
US 2002-353333P	P	20020201
US 2002-399673P	P	20020729
US 2002-434277P	P	20021217
WO 2003-US3022	W	20030131

OTHER SOURCE(S): MARPAT 139:164801
GI



I



II

AB Title compds. I [wherein L1 and L2 = independently a bond or a linker; R2 = (un)substituted alkyl, (hetero)cycloalkyl, or (hetero)aryl; R4 = H or R2; R5 = R6 or (un)substituted alkyl, alkenyl, or alkynyl; R6 = independently H, an electroneg. group, protected alc. or thiol, haloalkyl(oxy), halo, CN, NC, OCN, SCN, NO, NO2, N3, or (un)substituted

amino, sulfamoyl(oxy), acyl, carboxy, carbamoyl, (hetero)aryl(alkyl), etc.; with provisos and exclusions; and salts, hydrates, solvates, N-oxides, and prodrugs thereof] were prepared as inhibitors of the IgE and/or IgG receptor signaling cascades that lead to the release of chemical mediators. For example, coupling of 2,4-dichloropyrimidine with 4-ethoxyaniline in EtOH provided N2,N4-bis(4-ethoxyphenyl)-2,4-pyrimidinediamine (II). The latter inhibited degranulation of bone marrow derived mast cells challenged with anti-IgE and ionomycin with IC50 values of 4.5 μM and 4.4 μM, resp. Thus, I and their pharmaceutical compns. are useful in the treatment and prevention of diseases characterized by, caused by, or associated with the release of chemical mediators via degranulation of mast, basophil, neutrophil, or eosinophil cells and other processes effected by activation of the IgE and/or IgG receptor signaling cascades. The treatment and prevention of allergic diseases, low grade scarring, diseases associated with tissue destruction, diseases associated with tissue inflammation, inflammation, and scarring are targeted uses (no data).

IC ICM A61K

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

IT 40423-75-4P 40505-53-1P 312616-70-9P 312616-72-1P 313240-30-1P
313240-31-2P 313240-32-3P 313240-33-4P 313240-34-5P 313668-38-1P
313668-46-1P 325824-61-1P 325824-63-3P 362620-72-2P 439946-02-8P
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575477-38-2P 575477-39-3P 575477-40-6P 575477-41-7P 575477-42-8P
575477-43-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(IgE and/or IgG receptor modulator; preparation of pyrimidinediamines as IgE and/or IgG receptor modulators for treatment of allergic diseases, inflammatory conditions, and tissue destruction)

IT 575481-17-3P 575481-18-4P 575481-19-5P 575481-20-8P 575481-21-9P
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575484-34-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(IgE and/or IgG receptor modulator; preparation of pyrimidinediamines as IgE and/or IgG receptor modulators for treatment of allergic diseases, inflammatory conditions, and tissue destruction)

IT 51-21-8, 5-Fluorouracil 51-67-2, Tyramine 54-20-6, 5-Trifluoromethyluracil 55-81-2, 2-(4-Methoxyphenyl)ethylamine 56-41-7, L-Alanine, reactions **58-85-5**, D-(+)-Biotin 61-54-1, Tryptamine 64-04-0, 2-Aminoethylbenzene 65-49-6, 4-Amino-2-hydroxybenzoic acid 67-64-1, Acetone, reactions 75-31-0, Isopropylamine, reactions 77-92-9, Citric acid, reactions 78-96-6, 2-Hydroxypropylamine 88-19-7 89-57-6, 5-Amino-2-hydroxybenzoic acid 90-41-5, 2-Phenylaniline 91-00-9, 1,1-Diphenylmethylamine 95-76-1, 3,4-Dichloroaniline 95-80-7 96-32-2, Methyl bromoacetate 96-97-9, 2-Hydroxy-5-nitrobenzoic acid 98-16-8, 3-Trifluoromethylaniline 98-80-6, Phenylboronic acid 99-03-6, 3-Methylcarbonylaniline 99-05-8, 3-Aminobenzoic acid 99-09-2, 3-Nitroaniline 99-55-8, 2-Methyl-5-nitroaniline 99-57-0, 2-Amino-4-nitrophenol 99-59-2, 2-Methoxy-5-nitroaniline 99-88-7, 4-Isopropylaniline 99-98-9 100-02-7, 4-Nitrophenol, reactions 102-28-3 102-50-1, 4-Methoxy-2-methylaniline 103-71-9, Phenyl isocyanate, reactions 104-94-9, 4-Methoxyaniline 105-36-2, Ethyl bromoacetate 106-47-8, 4-Chloroaniline, reactions 106-49-0, 4-Methylaniline, reactions 106-50-3, 1,4-Diaminobenzene, reactions 107-10-8, n-Propylamine, reactions 107-11-9, Allylamine 108-42-9, 3-Chloroaniline 108-45-2, 3-Aminoaniline, reactions 108-91-8, Cyclohexylamine, reactions 109-01-3, N-Methylpiperazine 109-73-9, n-Butylamine, reactions 109-76-2, 1,3-Diaminopropane 109-81-9 109-83-1, N-Methyl-N-2-hydroxyethylamine 109-85-3, 2-Methoxyethylamine 109-90-0, Ethyl isocyanate 110-15-6, Succinic acid, reactions 110-16-7, Maleic acid, reactions 110-17-8, Fumaric acid, reactions 110-85-0, Piperazine, reactions 110-89-4, Piperidine, reactions 110-91-8, Morpholine, reactions 111-42-2, reactions 116-09-6 119-32-4, 4-Methyl-3-nitroaniline 121-90-4, 3-Nitrobenzoyl chloride 122-80-5, 4-Acetamidoaniline 123-30-8, 4-Hydroxyaniline 123-75-1, Pyrrolidine, reactions 124-68-5, 2-Amino-2-methylpropanol 135-95-5, 3-Hydroxymethyl-4-methoxyaniline 136-17-4 150-13-0, 4-Aminobenzoic acid 156-43-4, 4-Ethoxyaniline 156-87-6, 3-Hydroxypropylamine 320-51-4, 4-Chloro-3-trifluoromethylaniline 364-76-1, 4-Fluoro-3-nitroaniline 367-21-5, 3-Chloro-4-fluoroaniline 368-53-6 369-36-8, 2-Fluoro-5-nitroaniline 369-68-6, 3-(Trifluoromethylthio)aniline 371-40-4, 4-Fluoroaniline 372-16-7, 4-(Trifluoromethylthio)aniline 372-19-0, 3-Fluoroaniline 372-39-4, 3,5-Difluoroaniline 399-95-1, 2-Fluoro-4-hydroxyaniline 399-96-2, 3-Fluoro-4-hydroxyaniline 403-40-7 452-69-7, 4-Fluoro-3-methylaniline 452-84-6, 2-Fluoro-5-methylaniline 454-67-1, 3-Amino-5-fluorobenzotrifluoride 455-14-1, 4-Trifluoromethylaniline 459-73-4, Ethyl 2-aminoacetate 461-82-5, 4-Trifluoromethoxyaniline 462-08-8, 3-Aminopyridine 492-41-1, (1R,2S)-(-)-Norephedrine 501-53-1, Benzyl chloroformate 505-66-8, Homopiperazine 513-37-1, 1-Chloro-2-methylpropene 534-03-2, 2-Amino-1,3-propanediol 536-90-3, 3-Methoxyaniline 539-74-2, Ethyl 3-bromopropionate 540-51-2, 1-Bromo-2-hydroxyethane 554-84-7, 3-Nitrophenol 580-15-4, 6-Aminoquinoline 582-33-2, 3-Ethoxycarbonylaniline 589-16-2,

4-Ethylaniline 591-27-5, 3-Hydroxyaniline 593-51-1, Methylamine hydrochloride 600-00-0 611-08-5, 5-Nitrouracil 616-30-8, 3-Amino-1,2-propanediol 617-89-0, Furfurylamine 621-33-0, 3-Ethoxyaniline 623-04-1, 4-Aminobenzyl alcohol 623-33-6, Glycine ethyl ester hydrochloride 634-93-5, 2,4,6-Trichloroaniline 635-21-2, 2-Carboxy-4-chloroaniline 635-22-3, 4-Chloro-3-nitroaniline 695-34-1, 2-Amino-4-methylpyridine 720-01-4 765-30-0, Cyclopropylamine 765-39-9, 1-Aminopyrrole 769-92-6, 4-tert-Butylaniline 873-74-5, 4-Aminobenzonitrile 1009-36-5, 4-Chloro-3-methoxynitrobenzene 1072-98-6, 5-Chloro-2-aminopyridine 1080-06-4, L-Tyrosine methyl ester 1193-21-1, 4,6-Dichloropyrimidine 1462-37-9, 1-Benzyloxy-2-bromoethane 1476-23-9, Allyl isocyanate 1484-26-0, 3-Benzyloxyaniline 1535-73-5, 3-Trifluoromethoxyaniline 1535-76-8 1544-85-0 1603-41-4, 5-Methyl-2-aminopyridine 1673-47-8, 3-Chlorobenzohydrazide 1679-18-1, 4-Chlorophenylboronic acid 1687-53-2, 3-Hydroxy-4-methoxyaniline 1780-31-0, 2,4-Dichloro-5-methylpyrimidine 1780-40-1, 2,4,5,6-Tetrachloropyrimidine 1795-48-8, Isopropyl isocyanate 1798-11-4, 4-Nitrophenoxyacetic acid 1822-94-2, 5-(Chloromethyl)-3-phenyl-1,2,4-oxadiazole 1824-81-3, 2-Amino-6-methylpyridine 1877-77-6, 3-Aminobenzyl alcohol 1949-55-9 2038-03-1, 4-Morpholineethanamine 2144-37-8, Methyl 5-(chloromethyl)-2-furoate 2237-30-1, 3-Aminobenzonitrile 2243-47-2, 3-Phenylaniline 2393-17-1, 3-(p-Aminophenyl)propionic acid 2393-23-9, 4-Methoxybenzylamine 2423-71-4, 2,6-Dimethyl-4-nitrophenol 2516-47-4, Cyclopropylmethylamine 2524-67-6 2597-56-0, 2-Methoxy-4-nitrobenzoic acid 2620-50-0, Piperonylamine 2627-86-3 2666-93-5, Leucine methyl ester 2735-04-8, 2,4-Dimethoxyaniline 2743-60-4, L-Leucine ethyl ester 2835-78-1, 3-Phenylcarbonylaniline 2835-95-2, 3-Hydroxy-4-methylaniline 2835-96-3, 4-Hydroxy-3-methylaniline 2836-04-6, 3-(Dimethylamino)aniline 2949-22-6 3081-24-1 3096-69-3, 2,3-Dimethyl-4-hydroxyaniline 3096-71-7, 2,5-Dimethyl-4-hydroxyaniline 3182-93-2, L-Phenylalanine ethyl ester hydrochloride 3343-28-0, N-Phthaloyl-DL-glutamic anhydride 3544-25-0, 4-Cyanomethylaniline 3676-85-5, 4-Aminophthalimide 3731-51-9, 2-Pyridylmethylamine 3731-52-0, 3-Pyridylmethylamine 3764-01-0, 2,4,6-Trichloropyrimidine 3863-11-4, 3,4-Difluoroaniline 3886-69-9 3934-20-1, 2,4-Dichloropyrimidine 3964-52-1, 3-Chloro-4-hydroxyaniline 4152-09-4, N-Benzyl-1,2-diaminoethane 4344-55-2, 4-Butoxyaniline 4403-70-7, 3-Aminobenzylamine 4425-56-3, 5-Cyanouracil 4442-59-5, 2,3-Dihydro-1,4-benzodioxin-2-ylmethylamine 4461-30-7 4543-47-9, 3-Furanmethanamine 4553-21-3 4747-71-1, Cyclopentyl isocyanate 5071-96-5, 3-Methoxybenzylamine 5131-58-8 5192-03-0, 5-Aminoindole 5228-48-8 5292-43-3, tert-Butyl bromoacetate 5318-27-4, 6-Aminoindole 5345-54-0, 3-Chloro-4-methoxyaniline 5350-93-6 5369-16-4, 3-Isopropylaniline 5369-19-7, 3-tert-Butylaniline 5401-94-5 5428-54-6, 2-Methyl-5-nitrophenol 5438-70-0, Ethyl 4-aminophenyl acetate 5445-26-1, Ethyl 4-nitrophenylacetate 5683-33-0 5862-77-1, 3-Amino-4-ethoxyaniline 5930-28-9, 3,5-Dichloro-4-hydroxyaniline 5978-75-6, 9-Aminofluorene hydrochloride 6264-67-1 6299-85-0 6315-89-5, 3,4-Dimethoxyaniline 6358-64-1, 2,5-Dimethoxy-4-chloroaniline 6421-88-1 6628-77-9, 3-Amino-6-methoxypyridine 6967-12-0, 6-Aminoindazole 7568-93-6, 2-Amino-1-phenylethanol 7597-18-4 7647-01-0, Hydrochloric acid, reactions 7664-66-6, 4-Isopropoxyaniline 10242-12-3, 5-Nitro-2-benzofurancarboxylic acid 10272-07-8, 3,5-Dimethoxyaniline 13331-23-2, Furan-2-boronic acid 13871-68-6, 4-Acetoxyaniline 14268-66-7, 3,4-Methylenedioxyaniline 14415-44-2, 6-Aminocoumarin 16154-69-1, 4-(4-Benzylpiperazin-1-yl)aniline 16452-01-0, 3-Methoxy-4-methylaniline 16642-79-8, 3-(p-Nitrophenyl)propionic acid 16732-57-3 17413-10-4 17431-03-7, L-Valine ethyl ester 19293-62-0

19335-11-6, 5-Aminoindazole 19617-43-7, Ethoxycarbonyl isocyanate
20348-09-8, 2H-Pyrido[3,2-b]-1,4-oxazin-3(4H)-one 20734-67-2,
5-Aminobenzene-1,3-diol 21169-65-3 21443-96-9, 7-Aminoindazole
22013-33-8, 3,4-Ethylenedioxyaniline 22038-86-4, (R)-(+)-1-(4-
Methoxyphenyl)ethylamine 22235-25-2, 3-Methoxycarbonyl-5-
trifluoromethylaniline 24313-88-0, 3,4,5-Trimethoxyaniline 24358-62-1,
1-(4-Bromophenyl)ethylamine
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrimidinediamines as IgE and/or IgG receptor modulators for treatment of allergic diseases, inflammatory conditions, and tissue destruction)

IT 24424-99-5, Di-tert-butyl dicarbonate 25170-72-3 26215-14-5
26682-99-5, Phenylglycine methyl ester 27906-24-7 28020-37-3,
3-Amino-2,6-dimethoxypyridine 28059-69-0 28485-17-8,
5-Ethoxycarbonyluracil 28942-84-9 29263-94-3, Diethyl
2-bromo-2-methylmalonate 30418-59-8, 3-Aminophenylboronic acid
30734-81-7 30866-24-1 31329-64-3 33311-29-4 33786-89-9,
3-Amino-5-chloroaniline 33901-46-1 36082-50-5, 5-Bromo-2,4-
dichloropyrimidine 37045-73-1, 3-Methylsulfonylaminoaniline 38910-17-7
39811-17-1, 2-Methoxy-5-phenylaniline 39905-57-2, 4-n-Hexyloxyaniline
40353-34-2, 7-Nitro-1-tetralone 40615-04-1, Benzo[b]thiophene-3-
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(S)-(-)-1-(4-Methoxyphenyl)ethylamine 42758-84-9, 3-Acetoxyaniline
42923-79-5 42933-43-7, 5-Amino-2,3-dihydrobenzofuran 42961-88-6
50541-93-0, N-Benzyl-4-aminopiperidine 50593-24-3 50868-72-9,
5-Methoxy-2-methylaniline 50963-77-4 52481-41-1 52547-48-5
52913-11-8 53222-92-7 53250-82-1 54368-61-5 54962-75-3,
3-Bromo-5-trifluoromethylaniline 55411-44-4, 4-Amino-2-chloro-6-
methylphenol 55745-74-9 56607-76-2 56813-48-0 56932-44-6
56970-26-4, 4-Methoxy-3-phenylaniline 57319-65-0, 6-Amino-3,3-
dihydroisobenzofuran-1-one 57946-65-3 58754-71-5, 4-(2,3-
Dihydroxypropoxy)aniline 59954-04-0, Methyl 4-aminophenoxyacetate
62345-76-0 62802-42-0, 2-Chloro-5-fluoropyrimidine 63503-60-6,
3-Chlorophenylboronic acid 64628-73-5, 3-Chloro-4-
trifluoromethoxyaniline 65934-74-9, 4-Methyl-3-trifluoromethylaniline
66211-46-9, (R)-3-Amino-1,2-propanediol 67952-93-6, 3-Chloro-4-
methylbenzylamine 68621-88-5, 3-tert-Butoxycarbonylaminoaniline
69411-68-3, 3-Fluoro-4-trifluoromethylaniline 69959-88-2 70264-94-7,
Methyl (4-bromomethyl)-3-methoxybenzoate **70338-47-5**,
4-Benzyloxy-3-trifluoromethylaniline 71026-66-9, 4-tert-
Butoxycarbonylaminoaniline 71056-61-6 71597-85-8, 4-
Hydroxyphenylboronic acid 73732-51-1, 3-(Tetrazol-5-yl)aniline
80938-67-6 81720-19-6 87029-84-3 88327-91-7, 4-(Tetrahydro-(1H)-
pyrrol-1-ylsulfonyl)aniline 89260-46-8 89586-07-2 89976-75-0
92028-21-2 94839-07-3, 3,4-Methylenedioxyphenylboronic acid 96100-12-8
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-6, 4-[[3-(N-Morpholino)propyl]oxy]aniline 103361-43-9 105807-84-9,
6-Amino-2,2-dimethyl-4H-benzo[1,4]oxazin-3-one 110178-35-3 126874-73-5
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143071-39-0, 2-(2-Hydroxyethoxy)-5-nitropyridine 157837-31-5,
3-(1,3-Oxazol-5-yl)aniline 158196-47-5 167027-30-7 167756-90-3,
3-((N-tert-Butoxycarbonyl-N-methylamino)methyl)aniline 169286-84-4
173735-84-7 175136-34-2 175137-27-6 175201-62-4 175205-10-4
180258-45-1 189683-22-5 194025-85-9, 3-Methylaminocarbonyl-4-
methoxyaniline 195046-11-8 203664-68-0 203664-71-5 205117-39-1
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Butoxycarbonyl)aminomethyl]-4-methylaniline 220844-82-6 226571-61-5
280581-65-9 306934-74-7 306934-85-0 306937-22-4, Ethyl
1-(3-aminobenzyl)piperidine-4-carboxylate 307989-43-1 337463-65-7

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575473-25-5, 5-Amino-1-methylindazoline 575473-51-7 575473-75-5
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575482-94-9 575482-96-1 **575482-98-3** 575483-00-0
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575483-70-4 575483-77-1 575483-89-5 575483-91-9 575484-00-3
575484-02-5 575484-23-0 575484-55-8 575484-63-8 575484-64-9
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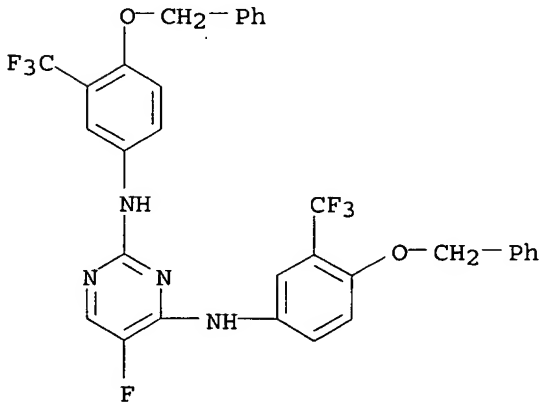
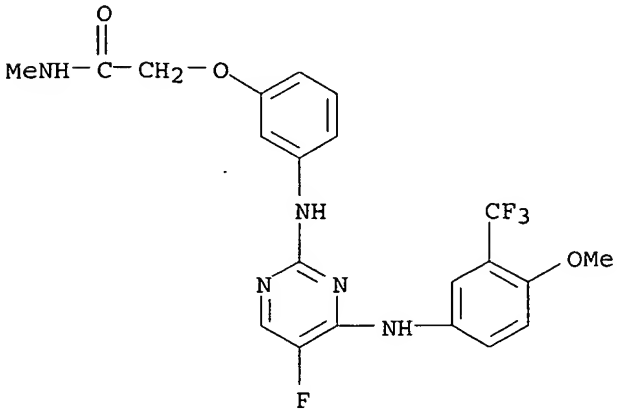
575485-10-8 575485-12-0 575485-27-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrimidinediamines as IgE and/or IgG receptor modulators for treatment of allergic diseases, inflammatory conditions, and tissue destruction)

IT **575476-23-2P 575482-97-2P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(IgE and/or IgG receptor modulator; preparation of pyrimidinediamines as IgE and/or IgG receptor modulators for treatment of allergic diseases, inflammatory conditions, and tissue destruction)

RN 575476-23-2 HCAPLUS
CN 2,4-Pyrimidinediamine, 5-fluoro-N,N'-bis[4-(phenylmethoxy)-3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

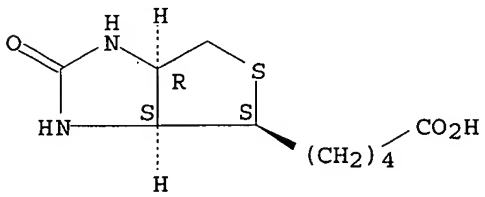


RN 575482-97-2 HCAPLUS
CN Acetamide, 2-[3-[[5-fluoro-4-[[4-methoxy-3-(trifluoromethyl)phenyl]amino]-2-pyrimidinyl]amino]phenoxy]-N-methyl- (9CI) (CA INDEX NAME)

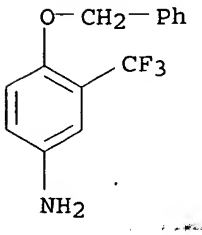


IT **58-85-5**, D-(+)-Biotin **70338-47-5**, 4-Benzyloxy-3-trifluoromethylaniline **575482-98-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrimidinediamines as IgE and/or IgG receptor modulators for treatment of allergic diseases, inflammatory conditions, and tissue destruction)
RN 58-85-5 HCAPLUS
CN 1H-Thieno[3,4-d]imidazole-4-pentanoic acid, hexahydro-2-oxo-, (3aS,4S,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

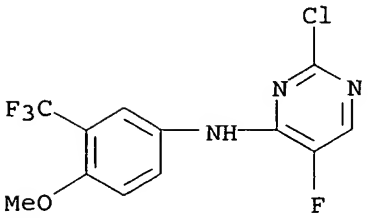


RN 70338-47-5 HCAPLUS
CN Benzenamine, 4-(phenylmethoxy)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 575482-98-3 HCAPLUS
CN 4-Pyrimidinamine, 2-chloro-5-fluoro-N-[4-methoxy-3-

(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



L33 ANSWER 6 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:190567 HCAPLUS
DOCUMENT NUMBER: 139:145678
TITLE: Activity-based fluorescent probes that target phosphatases
AUTHOR(S): Zhu, Qing; Huang, Xuan; Chen, Grace Y. J.; Yao, Shao Q.
CORPORATE SOURCE: Department of Chemistry, National University of Singapore, Singapore, 117543, Singapore
SOURCE: Tetrahedron Letters (2003), 44(13), 2669-2672
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:145678

AB We have successfully designed and synthesized two fluorescently-labeled, activity-based probes, Probe 1 and Probe 2, which were shown to label protein tyrosine phosphatases specifically, as well as other types of phosphatases. The probes were not reactive towards the other non-phosphatase enzymes tested. These probes may find potential applications in large-scale proteomic expts. whereby subclasses of proteins may be selectively identified.

CC 7-3 (Enzymes)

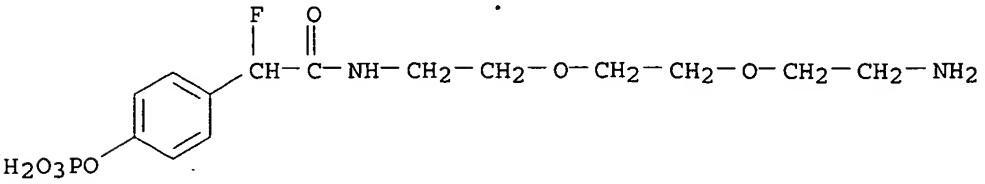
IT **570391-80-9DP**, conjugated with Cy3 **570391-81-0DP**, conjugated with Cy3
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(activity-based fluorescent probes that target phosphatases)

IT 97-51-8 107-15-3D, 1,2-Ethanediamine, conjugated with Cy3 108-30-5, reactions 298-12-4 814-49-3 929-59-9 38078-09-0, DAST **146368-16-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(activity-based fluorescent probes that target phosphatases)

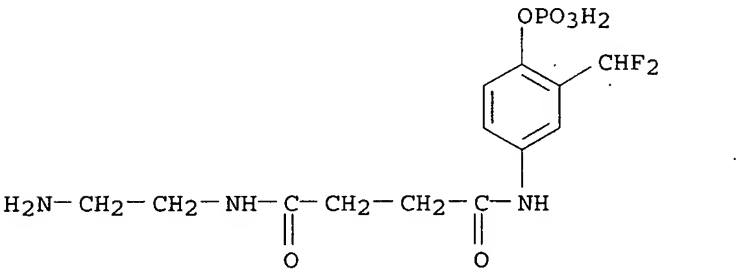
IT 1198-84-1P 150196-45-5P 153086-78-3P 182227-44-7P **182227-47-0P** 182227-50-5P **429692-36-4P** **429692-37-5P** **570391-82-1P** **570391-83-2P** **570391-84-3DP**, conjugated with Cy3 **648916-62-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(activity-based fluorescent probes that target phosphatases)

IT **570391-80-9DP**, conjugated with Cy3 **570391-81-0DP**, conjugated with Cy3
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(activity-based fluorescent probes that target phosphatases)

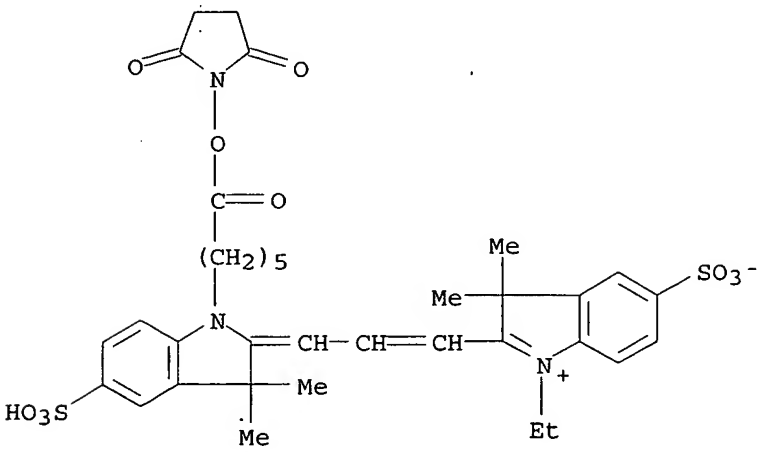
RN 570391-80-9 HCAPLUS
CN Benzeneacetamide, N-[2-[2-(2-aminoethoxy)ethoxy]ethyl]-α-fluoro-4-(phosphonooxy)- (9CI) (CA INDEX NAME)



RN 570391-81-0 HCAPLUS
CN Butanediamide, N-(2-aminoethyl)-N'-[3-(difluoromethyl)-4-(phosphonooxy)phenyl]- (9CI) (CA INDEX NAME)



IT **146368-16-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(activity-based fluorescent probes that target phosphatases)
RN 146368-16-3 HCAPLUS
CN 3H-Indolium, 2-[3-[1-[6-[(2,5-dioxo-1-pyrrolidinyl)oxy]-6-oxohexyl]-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene]-1-propenyl]-1-ethyl-3,3-dimethyl-5-sulfo-, inner salt (9CI) (CA INDEX NAME)

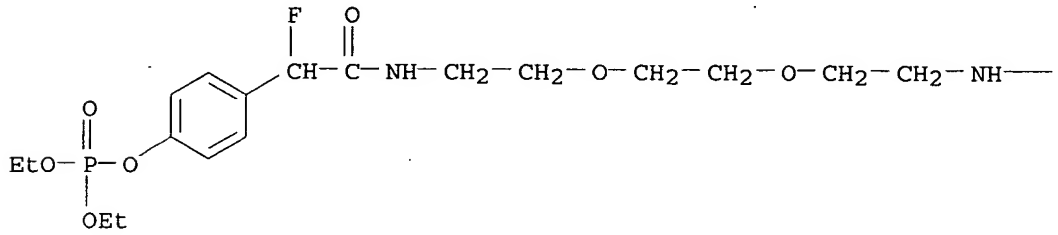


IT **182227-47-0P 429692-36-4P 429692-37-5P**

570391-82-1P 570391-83-2P 570391-84-3DP,
conjugated with Cy3 **648916-62-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(activity-based fluorescent probes that target phosphatases)

RN 182227-47-0 HCAPLUS
CN 5,8-Dioxa-2,11-diazatridecanoic acid, 13-[4-[(diethoxyphosphinyl)oxy]phenyl]-13-fluoro-12-oxo-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



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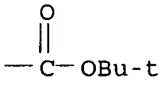
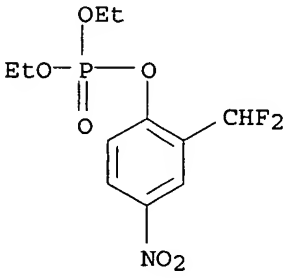
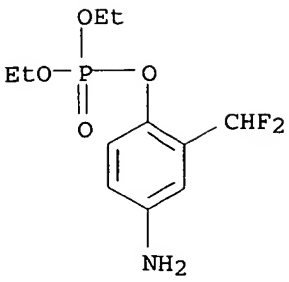


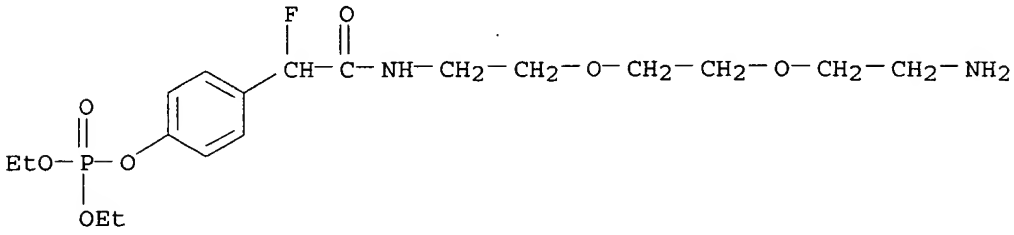
RN 429692-36-4 HCAPLUS
CN Phosphoric acid, 2-(difluoromethyl)-4-nitrophenyl diethyl ester (9CI) (CA INDEX NAME)



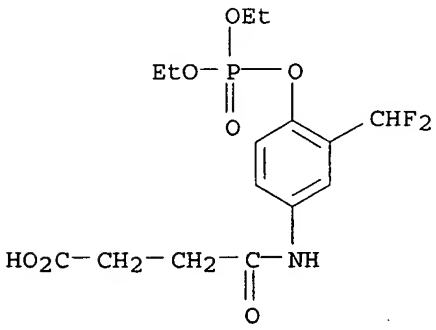
RN 429692-37-5 HCAPLUS
CN Phosphoric acid, 4-amino-2-(difluoromethyl)phenyl diethyl ester (9CI) (CA INDEX NAME)



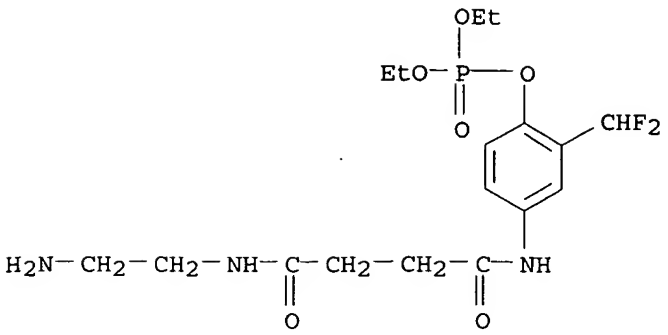
RN 570391-82-1 HCAPLUS
CN Phosphoric acid, 4-[2-[[2-[2-(2-aminoethoxy)ethoxy]ethyl]amino]-1-fluoro-2-oxoethyl]phenyl diethyl ester (9CI) (CA INDEX NAME)



RN 570391-83-2 HCAPLUS
CN Butanoic acid, 4-[[4-[(diethoxyphosphinyl)oxy]-3-(difluoromethyl)phenyl]amino]-4-oxo- (9CI) (CA INDEX NAME)

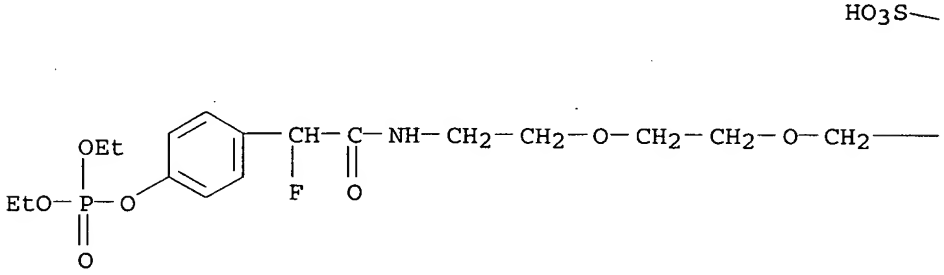


RN 570391-84-3 HCAPLUS
CN Phosphoric acid, 4-[[4-[(2-aminoethyl)amino]-1,4-dioxobutyl]amino]-2-(difluoromethyl)phenyl diethyl ester (9CI) (CA INDEX NAME)

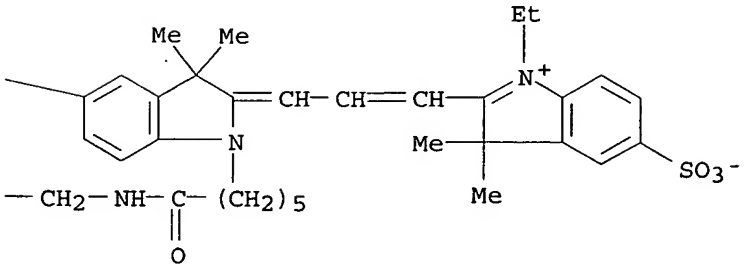


RN 648916-62-5 HCAPLUS
CN 3H-Indolium, 2-[3-[1-[18-[4-[(diethoxyphosphinyl)oxy]phenyl]-18-fluoro-6,17-dioxo-10,13-dioxa-7,16-diazaoctadec-1-yl]-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene]-1-propenyl]-1-ethyl-3,3-dimethyl-5-sulfo-, inner salt (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 7 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:133121 HCAPLUS
DOCUMENT NUMBER: 138:183234
TITLE: Conjugates of macrocyclic metal complexes with biomolecules, and the use thereof for producing agents

for use in NMR diagnosis, radiodiagnosis and radiotherapy

INVENTOR(S): Platzek, Johannes; Schmitt-Willich, Heribert; Michl, Guenther; Frenzel, Thomas; Suelzle, Detlev; Bauer, Hans; Raduechel, Bernd; Weinmann, Hanns-Joachim; Schirmer, Heiko

PATENT ASSIGNEE(S): Schering AG, Germany

SOURCE: PCT Int. Appl., 93 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003013617	A2	20030220	WO 2002-EP8000	20020718
WO 2003013617	A3	20040610		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10135355	C1	20030417	DE 2001-10135355	20010720
BR 2002011150	A	20040629	BR 2002-11150	20020718
EP 1450864	A2	20040901	EP 2002-794507	20020718
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
JP 2004536889	T2	20041209	JP 2003-518619	20020718
US 2003206865	A1	20031106	US 2002-198048	20020719

PRIORITY APPLN. INFO.: DE 2001-10135355 A 20010720
WO 2002-EP8000 W 20020718

OTHER SOURCE(S): MARPAT 138:183234

AB The invention discloses conjugates of macrocyclic metal complexes with biomols., as well as the production thereof. The conjugates are suited for use as contrast agents in NMR diagnosis and radiodiagnosis and as agents for radiotherapy. A high relaxivity is achieved and a fine tuning of the relaxivity is made possible by a special liganding of the macrocycles.

IC ICM A61K049-08
ICS A61K049-00

CC 8-9 (Radiation Biochemistry)
Section cross-reference(s): 28, 63, 78

IT **58-85-5D**, Biotin, derivs., conjugates 59-30-3D, Folic acid, conjugates 66-97-7D, Psoralen, conjugates 68-19-9D, Vitamin B12, conjugates 7429-91-6D, Dysprosium, complexes 7439-88-5D, Iridium, complexes 7439-89-6D, Iron, complexes 7439-92-1D, Lead, complexes 7439-94-3D, Lutetium, complexes 7439-96-5D, Manganese, complexes 7439-98-7D, Molybdenum, complexes 7440-00-8D, Neodymium, complexes 7440-02-0D, Nickel, complexes 7440-05-3D, Palladium, complexes 7440-10-0D, Praseodymium, complexes 7440-12-2D, Promethium, complexes 7440-15-5D, Rhenium, complexes 7440-17-7D, Rubidium, complexes 7440-18-8D, Ruthenium, complexes 7440-19-9D, Samarium, complexes 7440-20-2D, Scandium, complexes 7440-22-4D, Silver, complexes 7440-24-6D, Strontium, complexes 7440-26-8D, Technetium, complexes

7440-27-9D, Terbium, complexes 7440-30-4D, Thulium, complexes
7440-32-6D, Titanium, complexes 7440-45-1D, Cerium, complexes
7440-47-3D, Chromium, complexes 7440-48-4D, Cobalt, complexes
7440-50-8D, Copper, complexes 7440-52-0D, Erbium, complexes
7440-53-1D, Europium, complexes 7440-54-2D, Gadolinium, complexes
7440-55-3D, Gallium, complexes 7440-56-4D, Germanium, complexes
7440-60-0D, Holmium, complexes 7440-62-2D, Vanadium, complexes
7440-64-4D, Ytterbium, complexes 7440-65-5D, Yttrium, complexes
7440-69-9D, Bismuth, complexes 7440-74-6D, Indium, complexes
9001-67-6D, Neuraminidase, conjugates 33069-62-4D, Taxol, conjugates
51110-01-1D, Somatostatin, conjugates 52769-51-4D, Endoglycosidase, conjugates 69552-46-1D, Carbacyclin, conjugates 116243-73-3D, Endothelin, conjugates 127464-60-2D, Vascular endothelial growth factor, conjugates 189752-49-6D, Texaphyrin, conjugates 494750-83-3D, biomol. conjugates 494750-91-3D, biomol. conjugates 497922-13-1D, biomol. conjugates 497922-14-2D, biomol. conjugates
RL: DGN (Diagnostic use); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(macrocyclic metal complex-biomol. conjugates, preparation, and use as agents for NMR diagnosis, radiodiagnosis and radiotherapy)

IT 172744-88-6P 186095-25-0P 350588-09-9P **350588-10-2P**
350588-11-3P 494750-21-9P 494750-22-0P 494750-23-1P 494750-25-3P
494750-26-4P 494750-27-5P 494750-28-6P 494750-29-7P 494750-30-0P
494750-31-1P 494750-32-2P 494750-33-3P 494750-34-4P 494750-35-5P
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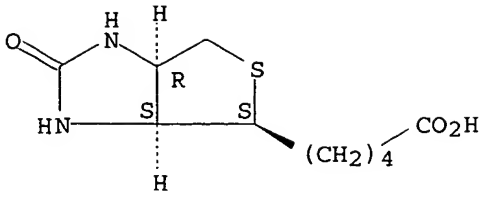
494750-46-8P 494750-47-9P 494750-48-0P 494750-49-1P 494750-53-7P
494750-55-9P 494750-57-1P 494750-59-3P 494750-60-6P 494750-62-8P
494750-64-0P **494750-65-1P** 494750-66-2P 494750-67-3P
494750-69-5P **494750-70-8P** 494750-71-9P 494750-72-0P
494750-74-2P 494750-76-4P 494750-78-6P 494750-80-0P 494750-82-2P
494750-84-4P 494750-85-5P 494750-87-7P 494750-89-9P 494750-90-2P
494750-92-4P 494750-93-5P 494750-94-6P 494750-95-7P 494750-96-8P
494750-97-9P 494750-98-0P 494750-99-1P 494751-00-7P 494751-01-8P
494751-02-9P 494751-03-0P 494751-04-1P 494751-05-2P 494751-06-3P
494751-07-4P 494751-09-6P 494751-10-9P 494751-11-0P 494751-12-1P
494751-13-2P 494751-14-3P 494751-15-4P 494751-16-5P 494751-17-6P
494751-18-7P 494751-19-8P 494751-20-1P 494751-21-2P 494751-22-3P
494751-23-4P 499203-20-2P 499203-21-3P 499203-22-4P 499203-23-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(macrocyclic metal complex-biomol. conjugates, preparation, and use as agents for NMR diagnosis, radiodiagnosis and radiotherapy)

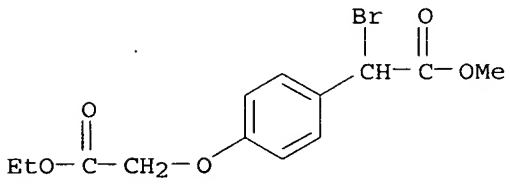
IT **58-85-5D**, Biotin, derivs., conjugates
RL: DGN (Diagnostic use); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(macrocyclic metal complex-biomol. conjugates, preparation, and use as agents for NMR diagnosis, radiodiagnosis and radiotherapy)

RN 58-85-5 HCAPLUS
CN 1H-Thieno[3,4-d]imidazole-4-pentanoic acid, hexahydro-2-oxo-, (3aS,4S,6aR)- (9CI) (CA INDEX NAME)

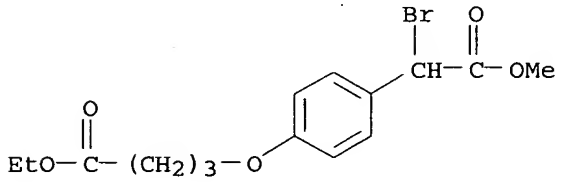
Absolute stereochemistry. Rotation (+).



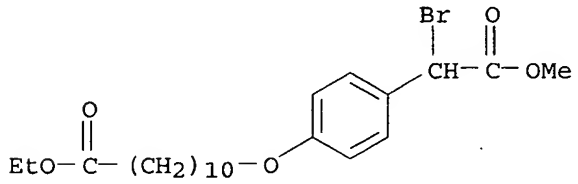
IT **350588-10-2P 494750-65-1P 494750-70-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(macrocyclic metal complex-biomol. conjugates, preparation, and use as agents for NMR diagnosis, radiodiagnosis and radiotherapy)
RN 350588-10-2 HCAPLUS
CN Benzeneacetic acid, α-bromo-4-(2-ethoxy-2-oxoethoxy)-, methyl ester (9CI) (CA INDEX NAME)



RN 494750-65-1 HCAPLUS
CN Benzeneacetic acid, α-bromo-4-(4-ethoxy-4-oxobutoxy)-, methyl ester (9CI) (CA INDEX NAME)



RN 494750-70-8 HCAPLUS
CN Benzeneacetic acid, α-bromo-4-[(11-ethoxy-11-oxoundecyl)oxy]-, methyl ester (9CI) (CA INDEX NAME)



L33 ANSWER 8 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:964313 HCAPLUS

DOCUMENT NUMBER: 138:55745
TITLE: Preparation of substituted 3-phenyl-2-alkoxypropanoic acids and analogs as modulators of peroxisome proliferator activated receptors for treatment of diabetes and related conditions
INVENTOR(S): Brooks, Dawn Alisa; Warshawsky, Alan M.; Montrose-Rafezadeh, Chahrzad; Reifel-Miller, Anne; Prieto, Lourdes; Rojo, Isabel; Martin, Jose Alfredo; Gonzales Garcia, Maria Rosario; Torrado, Alicia; Ferritto Crespo, Rafael; Lamas-Peteira, Carlos; Martin-Ortega Finger, Maria; Ardecky, Robert J.
PATENT ASSIGNEE(S): Eli Lilly and Company, USA; Ligand Pharmaceuticals Incorporated
SOURCE: PCT Int. Appl., 458 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002100813	A2	20021219	WO 2002-US16950	20020530
WO 2002100813	A3	20031127		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EE 200400001	A	20040216	EE 2004-1	20020530
EP 1392637	A2	20040303	EP 2002-739503	20020530
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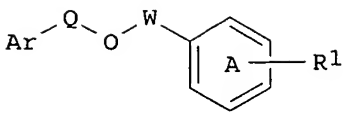
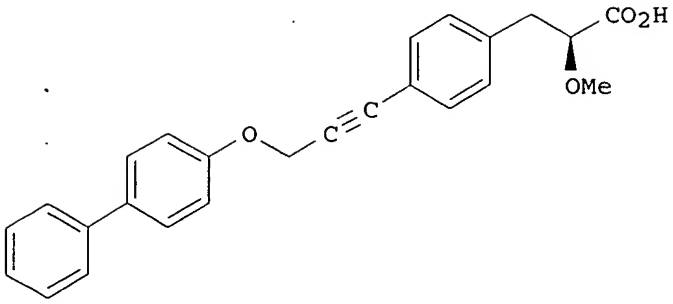
BR 2002010190	A	20040406	BR 2002-10190	20020530
PRIORITY APPLN. INFO.:			US 2001-297144P P	20010607
			WO 2002-US16950 W	20020530

OTHER SOURCE(S): MARPAT 138:55745
GI



I



II

AB Title compds. I [wherein Ar = (un)substituted aryl; Q = covalent bond, CH2, CH2CH2, CH2CH2CH2, or CH2CH2CH2CH2; W = (un)substituted (hetero)alkylene from 2-10 atoms in length in which 1 or more methylene groups have been replaced with CH=CH, C.tplbond.C, O, CO, NR7, NR7CO, C(=NOH), S, SO, SO2, or CHNR7R8; ring A is optionally substituted with up to 4 substituents in addition to R1; R1 = (CH2)nCH(OR2)(CH2)mE, CH=C(OR2)(CH2)mE, (CH2)nCHY(CH2)mE, or CH=CY(CH2)mE; E = CO2R3, alkylnitrile, carboxamide, or (un)substituted sulfonamide, acylsulfonamide, or tetrazole; R2 = H, haloalkyl, COR4, CO2R4, CONR5R6, CSR4, CSOR4, CSNR5R6, or (un)substituted aliphatic group, aralkyl, or aryl; Y = O, CH2, CH2CH2, or CH=CH bonded ortho to R1 on ring A; R3-R8 = independently H or (un)substituted aliphatic group or aryl; m and n = independently 0-2; or pharmaceutically acceptable salts, hydrates, stereoisomers, or solvates thereof] were prepared by solution phase and solid phase synthetic methods as peroxisome proliferator activated receptor (PPAR) modulators (no data). For example, (S)-2-methoxy-3-hydroxyphenylpropanoic acid Et ester was treated with Ph triflimide to give the 4-trifluoromethanesulfonyloxyphenyl derivative (97%). Substitution with propargyl alc. in the presence of PdCl2(PPh3)2 and TEA in DMF afforded the 4-(3-hydroxyprop-1-ynyl)phenyl intermediate (32%), which was coupled with 4-phenylphenol using the Mitsunobu procedure to give II. Binding and cotransfection studies showed that many of the compds. of the invention are selective PPARγ agonists or PPARα/PPARγ co-agonists (no data). Thus, I are useful for the treatment of hyperglycemia, dyslipidemia, Type I or II diabetes, hypertriglyceridemia, syndrome X, insulin resistance, heart failure, diabetic dyslipidemia, hyperlipidemia, hypercholesteremia, hypertension, obesity, anorexia bulimia, polycystic ovarian syndrome, anorexia nervosa, cardiovascular disease or other diseases where insulin resistance is a component (no data).

IC ICM C07C059-68
ICS C07C059-90; C07C059-72; C07C239-12; C07D311-30; C07D307-91; C07C219-10; C07D213-30; C07D215-14; C07D295-08; C07C217-94; A61K031-192; A61K031-195; A61P009-00; A61P003-04; A61P003-06; A61P003-00

CC 25-17 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1

IT 476436-68-7P, (2S)-2-Methoxy-3-[4-[3-(4-phenoxyphenoxy)propoxy]phenyl]propanoic acid 477979-23-0P, (2S)-2-Methoxy-3-[4-[3-(4-phenoxyphenoxy)prop-1-

ynyl]phenyl]propionic acid 477979-24-1P, (2S)-3-[4-[3-(4-Fluorophenoxy)prop-1-ynyl]phenyl]-2-methoxypropionic acid 477979-25-2P, (2S)-2-Methoxy-3-[4-[3-(3-phenylbenzofuran-6-yloxy)prop-1-ynyl]phenyl]propionic acid 477979-27-4P, (2S)-3-[4-[3-(4-Butylphenoxy)prop-1-ynyl]phenyl]-2-methoxypropionic acid 477979-28-5P, (2S)-2-Methoxy-3-[4-[3-[4-(4-trifluoromethylphenoxy)phenoxy]prop-1-ynyl]phenyl]propionic acid 477979-29-6P, (2S)-2-Methoxy-3-[4-[3-[(9-oxo-9H-fluoren-2-yl)oxy]prop-1-ynyl]phenyl]propionic acid 477979-30-9P, (2S)-2-Methoxy-3-[4-[3-[(4-oxo-2-phenyl-4H-chromen-7-yl)oxy]prop-1-ynyl]phenyl]propionic acid 477979-32-1P, (2S)-2-Methoxy-3-[4-[3-(3-phenylaminophenoxy)prop-1-ynyl]phenyl]propionic acid 477979-34-3P, (2S)-2-Methoxy-3-[4-[3-[(4-oxo-2-phenyl-4H-chromen-6-yl)oxy]prop-1-ynyl]phenyl]propionic acid 477979-35-4P, (2S)-3-[4-[3-[3-(4-Fluorophenyl)benzofuran-6-yloxy]prop-1-ynyl]phenyl]-2-methoxypropionic acid 477979-37-6P, (2S)-2-Methoxy-3-[4-[3-[4-(1-methyl-1-phenylethyl)phenoxy]prop-1-ynyl]phenyl]propionic acid 477979-38-7P, (2S)-2-Methoxy-3-[4-[3-[4-(phenylacetyl)phenoxy]prop-1-ynyl]phenyl]propionic acid 477979-39-8P, (2S)-3-[4-[3-(4-Benzylphenoxy)prop-1-ynyl]phenyl]-2-methoxypropionic acid 477979-40-1P, (2S)-3-[4-[3-[4-[(2-Fluorophenyl)hydroxyiminomethyl]phenoxy]prop-1-ynyl]phenyl]-2-methoxypropionic acid 477979-41-2P, (2S)-3-[4-[3-[4-[(Hydroxyimino)phenylmethyl)phenoxy]prop-1-ynyl]phenyl]-2-methoxypropionic acid 477979-42-3P, (2S)-3-[4-[3-[4-[(4-Fluorophenyl)hydroxyiminomethyl]phenoxy]prop-1-ynyl]phenyl]-2-methoxypropionic acid 477979-45-6P, (2S)-2-Methoxy-3-[4-[5-(4-phenoxyphenoxy)pent-1-ynyl]phenyl]propionic acid 477979-48-9P, (2S)-3-[4-[5-(4-Benzylphenoxy)pent-1-ynyl]phenyl]-2-methoxypropionic acid 477979-51-4P, (2S)-2-Methoxy-3-[4-[5-[4-(4-trifluoromethylphenoxy)phenoxy]pent-1-ynyl]phenyl]propionic acid 477979-52-5P, (2S)-2-Methoxy-3-[4-[5-[(4-oxo-2-phenyl-4H-chromen-7-yl)oxy]pent-1-ynyl]phenyl]propionic acid 477979-53-6P, (2S)-2-Methoxy-3-[4-[5-[(4-oxo-2-phenyl-4H-chromen-6-yl)oxy]pent-1-ynyl]phenyl]propionic acid 477979-54-7P, (2S)-2-Methoxy-3-[4-[5-[4-(1-methyl-1-phenylethyl)phenoxy]pent-1-ynyl]phenyl]propionic acid 477979-55-8P, (2S)-2-Methoxy-3-[4-[5-[(9-oxo-9H-fluoren-2-yl)oxy]pent-1-ynyl]phenyl]propionic acid 477979-56-9P, (2S)-2-Methoxy-3-[4-[5-(3-phenylaminophenoxy)pent-1-ynyl]phenyl]propionic acid 477979-58-1P, (2S)-2-Methoxy-3-[4-[5-(3-phenylbenzofuran-6-yloxy)pent-1-ynyl]phenyl]propionic acid 477979-59-2P, (2S)-3-[4-[5-[3-(4-Fluorophenyl)benzofuran-6-yloxy]pent-1-ynyl]phenyl]-2-methoxypropionic acid 477979-60-5P, (2S)-2-Methoxy-3-[4-[5-(4-phenylacetylphenoxy)pent-1-ynyl]phenyl]propionic acid 477979-61-6P, (2S)-3-[4-[5-(4-Butylphenoxy)pent-1-ynyl]phenyl]-2-methoxypropionic acid 477979-62-7P, (2S)-3-[4-[5-[4-[(2-Fluorophenyl)hydroxyiminomethyl]phenoxy]pent-1-ynyl]phenyl]-2-methoxypropanoic acid 477979-63-8P, (2S)-3-[4-[5-[4-[(4-Fluorophenyl)hydroxyiminomethyl]-phenoxy]pent-1-ynyl]phenyl]-2-methoxypropionic acid 477979-64-9P, (2S)-3-[4-[5-[4-[(Hydroxyimino)phenylmethyl]phenoxy]pent-1-ynyl]phenyl]-2-methoxypropionic acid 477979-65-0P, (2S)-3-[4-[4-(Biphenyl-4-yloxy)but-1-ynyl]phenyl]-2-methoxypropionic acid 477979-68-3P, (2S)-2-Methoxy-3-[4-[4-(4-phenoxyphenoxy)but-1-ynyl]phenyl]propionic acid 477979-73-0P, (2S)-3-[4-[4-[4-[(Hydroxyimino)phenylmethyl]phenoxy]but-1-ynyl]phenyl]-2-methoxypropionic acid 477979-74-1P, (2S)-3-[4-[4-[4-(4-Fluorobenzoyl)phenoxy]but-1-ynyl]phenyl]-2-methoxypropionic acid 477979-75-2P, (2S)-3-[4-[4-[3-(4-Fluorophenyl)benzofuran-6-yloxy]but-1-ynyl]phenyl]-2-methoxypropionic acid 477979-76-3P, (2S)-2-Methoxy-3-[4-[4-[4-(4-trifluoromethylphenoxy)phenoxy]but-1-ynyl]phenyl]propionic acid 477979-77-4P, (2S)-2-Methoxy-3-[4-[4-[(4-oxo-2-phenyl-4H-chromen-7-yl)oxy]but-1-ynyl]phenyl]propionic acid 477979-78-5P, (2S)-2-Methoxy-3-[4-[4-[(4-oxo-2-phenyl-4H-chromen-6-yl)oxy]but-1-

ynyl]phenyl]propionic acid 477979-82-1P, (2S)-3-[4-[6-(4-Benzoylphenoxy)hex-1-ynyl]phenyl]-2-methoxypropionic acid 477979-83-2P, (2S)-3-[4-[6-(Biphenyl-4-yloxy)hex-1-ynyl]phenyl]-2-methoxypropionic acid 477979-85-4P, (2S)-3-[4-[5-(4-Benzoylphenoxy)pentanoyl]phenyl]-2-methoxypropionic acid 477979-86-5P, (2S)-2-Methoxy-3-[4-[5-(4-phenoxyphenoxy)pentanoyl]phenyl]propionic acid 477979-87-6P, (2S)-3-[4-[4-(4-Benzoylphenoxy)butyryl]phenyl]-2-methoxypropionic acid 477979-89-8P, (2S)-2-Methoxy-3-[4-[4-(4-phenoxyphenoxy)butyryl]phenyl]propionic acid 477979-90-1P, (2S)-3-[4-[4-(Biphenyl-4-yloxy)butyryl]phenyl]-2-methoxypropionic acid 477979-91-2P, (2S)-3-[4-[6-(Biphenyl-4-yloxy)hexanoyl]phenyl]-2-methoxypropionic acid 477979-92-3P, (2S)-2-Methoxy-3-[4-[6-(4-phenoxyphenoxy)hexanoyl]phenyl]propionic acid 477979-93-4P, (2S)-3-[4-[6-(4-Benzoylphenoxy)hexanoyl]phenyl]-2-methoxypropionic acid 477979-94-5P, (2S)-3-[4-[5-(Biphenyl-4-yloxy)-1-(hydroxyimino)pentyl]phenyl]-2-methoxypropionic acid 477979-95-6P 477979-98-9P 477980-01-1P 477980-02-2P 477980-03-3P 477980-04-4P 477980-05-5P 477980-06-6P 477980-07-7P 477980-08-8P 477980-09-9P 477980-10-2P 477980-15-7P, (2S)-2-Methoxy-3-[4-[2-oxo-3-(4-phenoxyphenoxy)propoxy]phenyl]propionic acid 477980-16-8P, (2S)-2-Methoxy-3-[4-[3-(4-phenoxyphenoxymethyl)benzyloxy]phenyl]propionic acid 477980-17-9P, (2S)-2-Methoxy-3-[4-[2-(4-phenoxyphenoxymethyl)benzyloxy]phenyl]propionic acid 477980-18-0P, (2S)-2-Methoxy-3-[4-[3-(4-phenoxyphenoxy)phenoxy]phenyl]propionic acid 477980-19-1P, (2S)-3-[3'-(3-Benzoylphenoxymethyl)biphenyl-4-yl]-2-methoxypropionic acid 477980-21-5P, (2S)-3-[4'-(4-Benzoylphenoxymethyl)biphenyl-4-yl]-2-methoxypropionic acid 477980-25-9P 477980-26-0P 477980-27-1P 477980-28-2P 477980-29-3P 477980-30-6P 477980-34-0P 477980-39-5P 477980-40-8P 477980-41-9P 477980-42-0P, (2S)-3-[4-[3-(4-Benzoylphenoxy)propoxy]phenyl]-2-methoxypropionic acid 477980-47-5P, (2S)-3-[4-[3-(4-Benzylphenoxy)propoxy]phenyl]-2-methoxypropionic acid 477980-48-6P, (2S)-2-Methoxy-3-[4-[3-(3-phenylaminophenoxy)propoxy]phenyl]propionic acid 477980-49-7P, (2S)-3-[4-[3-(4-Butylphenoxy)propoxy]phenyl]-2-methoxypropionic acid 477980-50-0P, (2S)-3-[4-[3-[4-(2-Fluorobenzoyl)phenoxy]propoxy]phenyl]-2-methoxypropionic acid 477980-51-1P, (2S)-2-Methoxy-3-[4-[3-(9-oxo-9H-fluoren-2-yloxy)propoxy]phenyl]propionic acid 477980-52-2P, (2S)-2-Methoxy-3-[4-[3-[(2-methylbenzothiazol-5-yl)oxy]propoxy]phenyl]propionic acid 477980-53-3P, (2S)-2-Methoxy-3-[4-[3-[3-(morpholin-4-yl)phenoxy]propoxy]phenyl]propionic acid 477980-54-4P, (2S)-3-[4-[3-(Biphenyl-2-yloxy)propoxy]phenyl]-2-methoxypropionic acid 477980-55-5P, (2S)-3-[4-[2-(4-Benzoylphenoxy)ethoxy]phenyl]-2-methoxypropionic acid 477980-57-7P, (2S)-3-[4-[2-(Biphenyl-4-yloxy)ethoxy]phenyl]-2-methoxypropionic acid 477980-58-8P, (2S)-3-[4-[2-(Biphenyl-4-yloxy)acetyl]phenyl]-2-methoxypropionic acid 477980-62-4P, (2S)-2-Methoxy-3-[4-[2-(4-phenoxyphenoxy)acetyl]phenyl]propionic acid 477980-63-5P, (2S)-3-[4-[2-(4-Benzoylphenoxy)acetyl]phenyl]-2-methoxypropionic acid 477980-64-6P, (2S)-3-[4-[3-(Biphenyl-4-yloxy)propyl]phenyl]-2-methoxypropionic acid 477980-65-7P, (2S)-3-[4-[4-(Biphenyl-4-yloxy)butyl]phenyl]-2-methoxypropionic acid 477980-67-9P, (2S)-3-[4-[5-(Biphenyl-4-yloxy)pentyl]phenyl]-2-methoxypropionic acid 477980-68-0P, 3-[4-[3-(4-Benzoylphenoxy)propoxy]-3-methoxyphenyl]propionic acid 477980-73-7P, 3-[4-[3-[4-(4-Fluorobenzoyl)phenoxy]propoxy]-3-methoxyphenyl]-2-methoxypropionic acid 477980-75-9P, 3-[4-[3-(Biphenyl-4-yloxy)propoxy]-3-methoxyphenyl]-2-methoxypropionic acid 477980-78-2P, 2-Methoxy-3-[3-methoxy-4-[3-(4-phenoxyphenoxy)propoxy]phenyl]propionic acid 477980-79-3P, (2S)-3-[4-[3-(Biphenyl-4-yloxy)propoxy]-3-chlorophenyl]-2-methoxypropionic acid 477980-83-9P, 3-[4-[3-(Biphenyl-4-yloxy)propoxy]-3-fluorophenyl]-2-

methoxypropionic acid **477980-89-5P**, 3-[4-[3-(Biphenyl-4-yloxy)propoxy]-3-trifluoromethylphenyl]-2-methoxypropionic acid 477980-94-2P, (2S)-3-[6-[3-(Biphenyl-4-yloxy)propoxy]-4'-methoxybiphenyl-3-yl]-2-methoxypropionic acid 477980-98-6P, 3-[6-[3-(Biphenyl-4-yloxy)propoxy]-4'-fluorobiphenyl-3-yl]-2-methoxypropionic acid 477980-99-7P, 3-[4-[3-(Biphenyl-4-yloxy)propoxy]-2-methylphenyl]-2-methoxyacrylic acid 477981-03-6P, 3-[4-[3-(Biphenyl-4-yloxy)propoxy]-2-methylphenyl]-2-methoxypropionic acid 477981-05-8P, 3-[3-[3-(Biphenyl-4-yloxy)propoxy]phenyl]-2-methoxypropionic acid 477981-06-9P, 2-Methoxy-3-[3-[3-(4-phenoxyphenoxy)propoxy]phenyl]propionic acid 477981-08-1P, 3-[3-[3-(4-Benzoylphenoxy)propoxy]phenyl]-2-methoxypropionic acid 477981-10-5P, 2-Methoxy-3-[3-[5-(4-phenoxyphenoxy)pentyl]phenyl]propionic acid 477981-11-6P, (2S)-2-Methoxy-3-[4-[3-[4-[4-(piperidin-1-yl)benzoyl]phenoxy]propoxy]phenyl]propionic acid 477981-13-8P, (2S)-2-Methoxy-3-[4-[3-[4-[4-(morpholin-4-yl)benzoyl]phenoxy]propoxy]phenyl]propionic acid 477981-16-1P, (2S)-3-[4-[3-[4-[(Hydroxyimino)(4-hydroxyphenyl)methyl]phenoxy]propoxy]phenyl]-2-methoxypropionic acid 477981-17-2P, (2S)-3-[4-[3-(4-Benzoyl-3-hydroxyphenoxy)propoxy]phenyl]-2-methoxypropionic acid 477981-19-4P, (2S)-3-[4-[3-[4-(2,4-Dimethoxybenzoyl)phenoxy]propoxy]phenyl]-2-methoxypropionic acid 477981-22-9P, 3-[4-[3-(4-Benzylphenoxy)propoxy]-3-methoxyphenyl]-2-methoxypropionic acid 477981-24-1P, (S)-3-(4-Benzyloxyphenyl)-2-isopropoxypropionic acid 477981-29-6P, 2S-2-Isopropoxy-3-[4-[3-(4-phenoxyphenoxy)propoxy]phenyl]propanoic acid sodium salt 477981-35-4P 477981-37-6P, 3-[4-[3-(4-Butoxyphenoxy)propoxy]-3-methoxyphenyl]-2-methoxypropionic acid 477981-38-7P, 2-Methoxy-3-[3-methoxy-4-[3-(4-oxo-2-phenyl-4H-chromen-6-yloxy)propoxy]phenyl]propionic acid 477981-39-8P, 2-Methoxy-3-[3-methoxy-4-[3-[4-(4-trifluoromethylphenoxy)phenoxy]propoxy]phenyl]propionic acid 477981-40-1P, 3-[4-[3-(4-Benzyloxyphenoxy)propoxy]-3-methoxyphenyl]-2-methoxypropionic acid 477981-41-2P, 3-[4-[3-[4-(Dibenzofuran-3-yl)phenoxy]propoxy]-3-methoxyphenyl]-2-methoxypropionic acid 477981-43-4P, (2S)-3-[4-[4-(Biphenyl-4-yloxy)butoxy]phenyl]-2-methoxypropionic acid 477981-44-5P, (2S)-3-[4-[4-(4-Benzoylphenoxy)butoxy]phenyl]-2-methoxypropionic acid 477981-46-7P, (2S)-2-Methoxy-3-[4-[4-(4-phenoxyphenoxy)butoxy]phenyl]propionic acid 477981-47-8P, (2S)-2-Methoxy-3-[4-[2-(2,3,6-trifluorophenoxy)ethoxy]phenyl]propionic acid 477981-49-0P, (2S)-3-[4-(3-Benzyloxybenzyloxy)phenyl]-2-methoxypropionic acid 477981-52-5P, 3-[4-[3-(Biphenyl-4-yloxy)propoxy]-2-methoxyphenyl]-2-methoxypropionic acid 477981-54-7P, 3-[4-[3-(4-Benzoylphenoxy)propoxy]-2-methoxyphenyl]-2-methoxypropionic acid 477981-58-1P, 2-Methoxy-3-[2-methoxy-4-[3-(4-phenoxyphenoxy)propoxy]phenyl]propionic acid 477981-63-8P, 3-[2-Chloro-4-[3-(4-phenoxyphenoxy)propoxy]phenyl]-2-methoxypropionic acid 477981-67-2P, (2S)-4-[3-[4-(2-Carboxy-2-methyloxyethyl)phenoxy]propoxy]benzoic acid 477981-69-4P, (2S)-3-[4-[3-[4-(Dibenzothiophen-4-yl)phenoxy]propoxy]phenyl]-2-methoxypropanoic acid 477981-72-9P, (2S)-3-[4-[3-(4'-Hydroxybiphenyl-4-yloxy)propoxy]phenyl]-2-methoxypropionic acid 477981-73-0P, (2S)-4'-[3-[4-(2-Carboxy-2-methoxyethyl)phenoxy]propoxy]biphenyl-4-carboxylic acid 477981-74-1P 477981-75-2P 477981-76-3P, (2S)-3-[4-[3-[3-(4-Fluorophenyl)benzofuran-6-yloxy]propoxy]phenyl]-2-methoxypropionic acid 477981-77-4P, (2S)-2-Methoxy-3-[4-[3-(5,6,7,8-tetrahydronaphthalen-2-yloxy)propoxy]phenyl]propionic acid 477981-78-5P, (2S)-3-[4-[3-(4-Benzyloxyphenoxy)propoxy]phenyl]-2-methoxypropionic acid 477981-79-6P, (2S)-3-[4-[3-(4-Butoxyphenoxy)propoxy]phenyl]-2-methoxypropionic acid 477981-80-9P, (2S)-3-[4-[3-(4-Heptyloxyphenoxy)propoxy]phenyl]-2-methoxypropionic acid 477981-81-0P, (2S)-3-[4-[3-(6-Benzoylnaphthalen-2-yloxy)propoxy]phenyl]-2-methoxypropionic acid 477981-82-1P, (2S)-3-[4-[3-(Benzo[1,3]dioxol-5-

yloxy)propoxy]phenyl]-2-methoxypropionic acid 477981-83-2P, (2S)-3-[4-[3-(9H-Fluoren-2-yloxy)propoxy]phenyl]-2-methoxypropionic acid 477981-84-3P, (2S)-2-Methoxy-3-[4-[3-(4-octylphenoxy)propoxy]phenyl]propionic acid 477981-85-4P, (2S)-2-Methoxy-3-[4-[3-(naphthalen-1-yloxy)propoxy]phenyl]propionic acid 477981-86-5P, (2S)-3-[4-[3-(1H-Indol-7-yloxy)propoxy]phenyl]-2-methoxypropionic acid 477981-87-6P, (2S)-3-[4-[3-(4'-Fluorobiphenyl-4-yloxy)propoxy]phenyl]-2-methoxypropionic acid 477981-88-7P, (2S)-3-[4-[3-(4'-Chlorobiphenyl-4-yloxy)propoxy]phenyl]-2-methoxypropionic acid 477981-89-8P, (25S)-3-[4-[3-[3',5'-Bis(trifluoromethyl)biphenyl-4-yloxy]propoxy]phenyl]-2-methoxypropionic acid 477981-90-1P, (2S)-3-[4-[3-[4-(Dibenzofuran-4-yl)phenoxy]propoxy]phenyl]-2-methoxypropionic acid 477981-91-2P, (2S)-2-Methoxy-3-[4-[3-(4'-phenoxybiphenyl-4-yloxy)propoxy]phenyl]propionic acid 477981-92-3P, (2S)-2-Methoxy-3-[4-[3-[4-(thiophen-2-yl)phenoxy]propoxy]phenyl]propionic acid 477981-93-4P, (2S)-3-[4-[3-(3'-Chlorobiphenyl-4-yloxy)propoxy]phenyl]-2-methoxypropionic acid 477981-94-5P, (2S)-3-[4-[3-(2'-Chlorobiphenyl-4-yloxy)propoxy]phenyl]-2-methoxypropionic acid 477981-95-6P, (2S)-3-[4-[3-(2'-Fluorobiphenyl-4-yloxy)propoxy]phenyl]-2-methoxypropionic acid 477981-96-7P, (2S)-3-[4-[3-[4-(Benzo[1,3]dioxol-5-yl)phenoxy]propoxy]phenyl]-2-methoxypropionic acid 477981-97-8P, (2S)-3-[4-[3-(4'-tert-Butylbiphenyl-4-yloxy)propoxy]phenyl]-2-methoxypropionic acid 477981-98-9P, (2S)-2-Methoxy-3-[4-[3-[3'-(trifluoromethoxy)biphenyl-4-yloxy]propoxy]phenyl]propionic acid 477981-99-0P, (2S)-2-Methoxy-3-[4-[3-[4'-(trifluoromethoxy)biphenyl-4-yloxy]propoxy]phenyl]propionic acid 477982-00-6P, (2S)-3-[4-[3-[4-(2-Chlorobenzoylamino)phenoxy]propoxy]phenyl]-2-methoxypropionic acid 477982-01-7P, (2S)-2-Methoxy-3-[4-[3-[4-(2-methoxybenzoylamino)phenoxy]propoxy]phenyl]propionic acid 477982-02-8P, (2S)-3-[4-[3-[4-(2,2-Dimethylpropionylamino)phenoxy]propoxy]phenyl]-2-methoxypropionic acid 477982-03-9P, (2S)-3-[4-[3-[4-(3-Fluorobenzoylamino)phenoxy]propoxy]phenyl]-2-methoxypropionic acid 477982-04-0P, (2S)-2-Methoxy-3-[4-[3-[4-(3-methoxybenzoylamino)phenoxy]propoxy]phenyl]propionic acid 477982-05-1P, (2S)-2-Methoxy-3-[4-[3-[4-(3-methylbenzoylamino)phenoxy]propoxy]phenyl]propionic acid 477982-06-2P, (2S)-3-[4-[3-[4-(4-Fluorobenzoylamino)phenoxy]propoxy]phenyl]-2-methoxypropionic acid 477982-07-3P, (2S)-3-[4-[3-[4-(4-Chlorobenzoylamino)phenoxy]propoxy]phenyl]-2-methoxypropionic acid 477982-08-4P, (2S)-2-Methoxy-3-[4-[3-[4-(4-methoxybenzoylamino)phenoxy]propoxy]phenyl]propionic acid 477982-09-5P 477982-10-8P, (2S)-3-[4-[3-[4-(2-Chlorobenzoyl)phenoxy]propoxy]phenyl]-2-methoxypropionic acid 477982-11-9P, (2S)-2-Methoxy-3-[4-[3-[4-(naphthalene-1-carbonyl)phenoxy]propoxy]phenyl]propionic acid 477982-12-0P, (2S)-3-[4-[3-[4-(3-Fluorobenzoyl)phenoxy]propoxy]phenyl]-2-methoxypropionic acid 477982-13-1P, (2S)-2-Methoxy-3-[4-[3-[4-(3-methoxybenzoyl)phenoxy]propoxy]phenyl]propionic acid 477982-14-2P, (2S)-2-Methoxy-3-[4-[3-[4-(naphthalene-2-carbonyl)phenoxy]propoxy]phenyl]propionic acid 477982-15-3P, (2S)-2-Methoxy-3-[4-[3-[4-(4-methylbenzoyl)phenoxy]propoxy]phenyl]propionic acid 477982-16-4P, (2S)-3-[4-[3-[4-(2,2-Dimethylpropionyl)phenoxy]propoxy]phenyl]-2-methoxypropionic acid 477982-17-5P, (2S)-3-[4-[3-(4-Isobutyrylphenoxy)propoxy]phenyl]-2-methoxypropionic acid 477982-18-6P, (2S)-2-Methoxy-3-[4-[3-[4-(3-phenylpropionyl)phenoxy]propoxy]phenyl]propionic acid 477982-19-7P, 3-[4-[3-(Biphenyl-4-yloxy)propoxy]-2-fluorophenyl]-2-methoxypropionic acid 477982-23-3P, 2-Phenoxy-3-[4-[3-(4-phenoxyphenoxy)propoxy]phenyl]propanoic acid 477982-26-6P 477982-31-3P, (2S)-2-Methoxy-3-[4-[2-methyl-3-(4-phenoxyphenoxy)propoxy]phenyl]propionic acid 477982-34-6P, (2S)-3-[4-(3-Benzyloxypropoxy)phenyl]-2-methoxypropionic acid 477982-35-7P 477982-36-8P, (2S)-2-Ethoxy-3-[4-[3-(4-

phenoxyphenoxy)propoxy]phenyl]propionic acid 477982-39-1P, (2S)-2-Benzyloxy-3-[4-[3-(4-phenoxyphenoxy)propoxy]phenyl]propionic acid 477982-43-7P, (2S)-3-[4-[3-[4-[4-(2-Hydroxyethoxy)benzoyl]phenoxy]propoxy]phenyl]-2-methoxypropionic acid 477982-44-8P, (2S)-3-[4-[3-(4-Phenoxyphenoxy)propoxy]phenyl]-2-propoxypropionic acid 477982-48-2P, (2S)-3-[4-[3-(4-Benzoylphenoxy)propoxy]phenyl]-2-ethoxypropionic acid 477982-50-6P, (2S)-3-[4-[3-(4-Benzylphenoxy)propoxy]phenyl]-2-ethoxypropionic acid 477982-52-8P, (2S)-3-[4-[3-(4-Benzoylphenoxy)propoxy]-3-chlorophenyl]-2-ethoxypropionic acid 477982-55-1P, (2S)-4'-[3-[4-(2-Carboxy-2-methoxyethyl)-2-methoxyphenoxy]propoxy]biphenyl-4-carboxylic acid 477982-58-4P, (2S)-3-[4-[3-(4'-tert-Butylbiphenyl-4-yloxy)propoxy]-2-methoxyphenyl]-2-methoxypropionic acid 477982-62-0P, (2S)-3-[4-[3-[4-(4-Hydroxyphenoxy)phenoxy]propoxy]phenyl]-2-methoxypropionic acid 477982-63-1P, (2S)-2-Methoxy-3-[4-[3-[4-(2,2,3,3-tetrafluoropropoxy)phenoxy]propoxy]phenyl]propionic acid 477982-67-5P, (2S)-2-Methoxy-3-[4-[3-[4-(3-methylbutoxy)phenoxy]propoxy]phenyl]propionic acid 477982-71-1P, (2S)-3-[4-[3-(4-Isobutoxyphenoxy)propoxy]phenyl]-2-methoxypropionic acid 477982-72-2P, (2S)-3-[4-[3-(4-Isopropoxyphenoxy)propoxy]phenyl]-2-methoxypropionic acid 477982-73-3P , (2S)-3-[4-[3-(4-Cyclohexylmethoxyphenoxy)propoxy]phenyl]-2-methoxypropionic acid 477982-74-4P, (2S)-2-Methoxy-3-[4-[3-(4-phenethyloxyphenoxy)propoxy]phenyl]propionic acid 477982-75-5P, (2S)-3-[4-[3-[4-(3-Dimethylaminopropoxy)phenoxy]propoxy]phenyl]-2-methoxypropionic acid 477982-76-6P, (2S)-3-[4-[3-(4-Carboxymethoxyphenoxy)propoxy]phenyl]-2-methoxypropionic acid 477982-77-7P, (2S)-3-[4-[3-[4-(1H-Indol-5-yl)phenoxy]propoxy]phenyl]-2-methoxypropionic acid 477982-80-2P, (2S)-2-Methoxy-3-[4-[3-[4-(pyridin-3-yl)phenoxy]propoxy]phenyl]propionic acid 477982-81-3P, (2S)-2-Methoxy-3-[4-[3-[4-(pyridin-4-yl)phenoxy]propoxy]phenyl]propionic acid 477982-82-4P, (2S)-2-Methoxy-3-[4-[3-[4-(quinolin-8-yl)phenoxy]propoxy]phenyl]propionic acid 477982-83-5P, (2S)-3-[4-[3-(4'-Cyanobiphenyl-4-yloxy)propoxy]phenyl]-2-methoxypropionic acid 477982-85-7P, (2S)-2-Methoxy-3-[4-[3-[[4'-(1H-tetrazol-5-yl)biphenyl-4-yl]oxy]propoxy]phenyl]propionic acid 477982-87-9P, (2S)-3-[4-[3-[4-(Imidazol-1-yl)phenoxy]propoxy]phenyl]-2-methoxypropionic acid 477982-88-0P, (2S)-3-[4-[3-[4-(1,3-Dioxo-1,3-dihydroisoindol-2-yl)phenoxy]propoxy]phenyl]-2-methoxypropionic acid 477982-89-1P, (2S)-3-[4-[3-[4-(4-Acetylpiperazin-1-yl)phenoxy]propoxy]phenyl]-2-methoxypropionic acid 477982-90-4P, (2S)-2-Methoxy-3-[4-[3-[4-(piperazin-1-yl)phenoxy]propoxy]phenyl]propionic acid 477982-92-6P, (2S)-2-Methoxy-3-[4-[3-[4-(morpholin-4-yl)phenoxy]propoxy]phenyl]propionic acid 477982-96-0P, 3-[4-[3-(4-Benzoylphenoxy)propoxy]-2-chlorophenyl]-2-ethoxypropionic acid 477982-98-2P, (2S)-2-Methoxy-3-[4-[3-(3-trifluoromethylphenoxy)propoxy]phenyl]propionic acid 477982-99-3P, (2S)-2-Methoxy-3-[4-(3-phenoxypropoxy)phenyl]propionic acid 477983-00-9P, (2S)-3-[4-[3-(Biphenyl-3-yloxy)propoxy]phenyl]-2-methoxypropionic acid 477983-01-0P, 2-Methoxy-3-[4-[2-(4-phenoxyphenoxy)ethoxy]phenyl]propionic acid 477983-08-7P, (2S)-3-[4-[3-(2-Cyanophenoxy)propoxy]phenyl]-2-methoxypropionic acid 477983-09-8P, (2S)-2-Methoxy-3-[4-[3-(2-methoxyphenoxy)propoxy]phenyl]propionic acid 477983-10-1P, (S)-2-[3-[4-(2-Carboxy-2-methoxyethyl)phenoxy]propoxy]benzoic acid 477983-11-2P, (2S)-3-[4-[3-(3-Cyanophenoxy)propoxy]phenyl]-2-methoxypropionic acid 477983-12-3P, (2S)-3-[4-[3-(3-Dimethylaminophenoxy)propoxy]phenyl]-2-methoxypropionic acid 477983-13-4P, (2S)-3-[3-[4-(2-Carboxy-2-methoxyethyl)phenoxy]propoxy]benzoic acid 477983-14-5P, (2S)-3-[4-[3-[(Indan-5-yl)oxy]propoxy]phenyl]-2-methoxypropionic acid 477983-15-6P, (2S)-2-Methoxy-3-[4-[3-(naphthalen-2-

yloxy)propoxy]phenyl]propionic acid 477983-16-7P, (2S)-3-[4-[3-(1H-Indol-5-yloxy)propoxy]phenyl]-2-methoxypropionic acid 477983-17-8P, (2S)-2-Methoxy-3-[4-[3-(quinolin-6-yloxy)propoxy]phenyl]propionic acid 477983-18-9P, (2S)-2-Methoxy-3-[4-[3-(3-methoxyphenoxy)propoxy]phenyl]propionic acid 477983-19-0P, (2S)-3-[4-[3-(3-Fluorophenoxy)propoxy]phenyl]-2-methoxypropionic acid
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(PPAR modulator; preparation of substituted (phenyl)(alkoxy)propanoic acids and analogs as PPAR modulators for treatment of diabetes and related conditions)

IT 348-27-6P, 2-Fluoro-4-hydroxybenzaldehyde 405-05-0P, 3-Fluoro-4-hydroxybenzaldehyde 627-18-9P, 3-Bromopropan-1-ol 1073-05-8P, [1,3,2]Dioxathiane 2,2-dioxide 2973-78-6P, 3-Bromo-4-hydroxybenzaldehyde 3351-60-8P, 4-(2-Bromoethoxy)biphenyl 16251-33-5P, 1-Bromo-3-(4-phenoxyphenyl)propane 19070-95-2P, 2-(Biphenyl-4-yloxy)ethanol 23418-85-1P, Toluene-4-sulfonic acid but-3-ynyl ester 29169-19-5P 54334-74-6P, (Biphenyl-4-yloxy)acetic acid ethyl ester 63457-51-2P, 1-(3-Bromopropoxy)-4-phenoxybenzene 69455-12-5P, 4-Benzyloxy-3-bromobenzaldehyde 87545-48-0P, 4-(2-Bromoethoxy)phenoxybenzene 96363-80-3P, Methanesulfonic acid 3-dimethylaminopropyl ester 102229-10-7P, 2-(tert-Butyldimethylsilanyloxy)ethanol 111915-33-4P, 4-(2,2,3,3-Tetrafluoropropoxy)phenol 113795-28-1P, 4-(3-Bromopropoxy)biphenyl 119437-35-3P, 1-Chloro-3-(4-phenoxyphenyl)propane 128316-64-3P, 3-(4-Benzyloxyphenyl)-2-hydroxypropanoic acid methyl ester 156335-14-7P, Methyl 3-(4-hydroxyphenyl)-2-methoxypropanoate 156335-15-8P, 2-Ethoxy-3-(4-hydroxyphenyl)propionic acid methyl ester 156659-87-9P, (2S,4S)-4-(tert-Butyldimethylsilanyloxy)pentan-2-ol 162919-37-1P 173025-78-0P, 3-(Biphenyl-4-yloxy)propan-1-ol 183612-97-7P, (1R*,3S*)-3-(tert-Butyldimethylsilanyloxy)cyclopentanol 183795-20-2P, trans-3-(tert-Butyldimethylsilanyloxy)cyclopentanol 211617-68-4P 222835-03-2P, 3-(4-Benzyloxyphenyl)-2-ethoxyacrylic acid ethyl ester 223126-28-1P, 3-(4-Benzyloxyphenyl)-2-ethoxypropionic acid ethyl ester 251978-39-9P, 3-(4-Hydroxyphenyl)-2-phenoxypropanoic acid methyl ester 267228-40-0P, (S)-3-(4-Benzyloxyphenyl)-2-hydroxypropionic acid ethyl ester 267228-41-1P, (2S)-2-Hydroxy-3-(4-hydroxyphenyl)propionic acid ethyl ester 325827-53-0P, (S)-3-(4-Hydroxyphenyl)-2-isopropoxypropionic acid ethyl ester 361576-28-5P, 3-(4-Benzyloxyphenyl)-2-ethoxy-3-hydroxypropionic acid ethyl ester 477979-19-4P, (2S)-2-Methoxy-3-(4-trifluoromethanesulfonyloxyphenyl)propionic acid ethyl ester 477979-21-8P, (2S)-3-[4-(3-Hydroxyprop-1-ynyl)phenyl]-2-methoxypropionic acid ethyl ester 477979-26-3P, (2S)-3-[4-(3-Chloroprop-1-ynyl)phenyl]-2-methoxypropionic acid ethyl ester 477979-44-5P, (2S)-3-[4-(5-Hydroxypent-1-ynyl)phenyl]-2-methoxypropionic acid ethyl ester 477979-49-0P, 3-[4-(5-Bromopent-1-ynyl)phenyl]-2-methoxypropionic acid ethyl ester 477979-66-1P, 4-But-3-ynyloxybiphenyl 477979-67-2P, (2S)-3-[4-[4-(Biphenyl-4-yloxy)but-1-ynyl]phenyl]-2-methoxypropionic acid ethyl ester 477979-69-4P, 1-(But-3-ynyloxy)-4-phenoxybenzene 477979-71-8P, [4-(But-3-ynyloxy)phenyl]phenylmethanone 477979-72-9P, (2S)-3-[4-[4-(4-Benzoylphenoxy)but-1-ynyl]phenyl]-2-methoxypropionic acid ethyl ester 477979-80-9P, (2S)-3-[4-(6-Hydroxyhex-1-ynyl)phenyl]-2-methoxypropionic acid ethyl ester 477979-88-7P, (2S)-3-[4-[4-(4-Benzoylphenoxy)butyryl]phenyl]-2-methoxypropionic acid ethyl ester 477979-96-7P, cis-2-(tert-Butyldimethylsilanyloxy)cyclopentanol 477979-97-8P 477979-99-0P 477980-00-0P 477980-11-3P, (2R,3S)-3-(4-Phenoxyphenoxy)butan-2-ol 477980-12-4P 477980-13-5P 477980-20-4P, (2S)-3-(3'-Hydroxymethylbiphenyl-4-yl)-2-methoxypropionic

acid ethyl ester 477980-23-7P 477980-24-8P 477980-35-1P
477980-36-2P, 3-(Biphenyl-4-yloxy)cyclohexanol 477980-37-3P,
(trans)-3-(Biphenyl-4-yloxy)cyclohexanol 477980-38-4P,
(cis)-3-(Biphenyl-4-yloxy)cyclohexanol 477980-44-2P,
(2S)-3-[4-(tert-Butyldimethylsilanyloxy)phenyl]-2-methoxypropionic acid
477980-45-3P, (2S)-3-[4-(3-Hydroxypropoxy)phenyl]-2-methoxypropionic acid
477980-56-6P, (2S)-3-[4-(2-Hydroxyethoxy)phenyl]-2-methoxypropanoic acid
477980-59-9P, (2S)-3-(4-Ethynylphenyl)-2-methoxypropionic acid ethyl ester
477980-60-2P, (2S)-3-(4-Acetylphenyl)-2-methoxypropionic acid ethyl ester
477980-61-3P, (2S)-3-[4-(2-Bromoacetyl)phenyl]-2-methoxypropionic acid
ethyl ester 477980-66-8P, (2S)-3-[4-(4-Hydroxybutyl)phenyl]-2-
methoxypropionic acid ethyl ester 477980-69-1P, 3-(4-Benzyloxy-3-
methoxyphenyl)-3-hydroxy-2-methoxypropionic acid methyl ester
477980-70-4P, 3-(4-Hydroxy-3-methoxyphenyl)-2-methoxypropionic acid methyl
ester 477980-71-5P, 3-(4-Hydroxy-3-methoxyphenyl)-2-methoxypropionic
acid 477980-72-6P, 3-[4-(tert-Butyldimethylsilanyloxy)-3-methoxyphenyl]-
2-methoxypropionic acid 477980-76-0P, 3-(4-Hydroxy-3-methoxyphenyl)-2-
methoxypropionic acid ethyl ester 477980-77-1P, 3-[4-[3-(Biphenyl-4-
yloxy)propoxy]-3-methoxyphenyl]-2-methoxypropionic acid ethyl ester
477980-80-6P, (2S)-3-(3-Chloro-4-hydroxyphenyl)-2-methoxypropionic acid
ethyl ester 477980-82-8P, (2S)-3-[4-[3-(Biphenyl-4-yloxy)propoxy]-3-
chlorophenyl]-2-methoxypropionic acid ethyl ester 477980-84-0P,
2-(3-Fluoro-4-methoxyphenyl)-[1,3]dioxolane 477980-85-1P,
4-[1,3]Dioxolan-2-yl-2-fluorophenol 477980-86-2P, 4-[3-(Biphenyl-4-
yloxy)propoxy]-3-fluorobenzaldehyde 477980-87-3P, 3-[4-[3-(Biphenyl-4-
yloxy)propoxy]-3-fluorophenyl]-3-hydroxy-2-methoxypropionic acid methyl
ester 477980-88-4P, 3-[4-[3-(Biphenyl-4-yloxy)propoxy]-3-fluorophenyl]-2-
methoxypropionic acid methyl ester **477980-90-8P**,
4-Benzyloxy-3-trifluoromethylbenzaldehyde 477980-91-9P,
3-(4-Hydroxy-3-trifluoromethylphenyl)-2-methoxyacrylic acid methyl ester
477980-92-0P, 3-[4-[3-(Biphenyl-4-yloxy)propoxy]-3-
trifluoromethylphenyl]-2-methoxyacrylic acid methyl ester
477980-93-1P, 3-[4-[3-(Biphenyl-4-yloxy)propoxy]-3-
trifluoromethylphenyl]-2-methoxyacrylic acid 477980-95-3P
477980-96-4P, (2S)-3-(6-Hydroxy-4'-methoxybiphenyl-3-yl)-2-
methoxypropionic acid ethyl ester 477980-97-5P, (2S)-3-[6-[3-(Biphenyl-4-
yloxy)propoxy]-4'-methoxybiphenyl-3-yl]-2-methoxypropionic acid ethyl
ester 477981-00-3P, 2-Methyl-4-(triisopropylsilanyloxy)benzaldehyde
477981-01-4P, 3-[4-[3-(Biphenyl-4-yloxy)propoxy]-2-methylphenyl]-2-
methoxyacrylic acid methyl ester 477981-02-5P, 3-(4-Hydroxy-2-
methylphenyl)-2-methoxyacrylic acid 477981-04-7P, 3-[4-[3-(Biphenyl-4-
yloxy)propoxy]-2-methylphenyl]-2-methoxypropionic acid methyl ester
477981-07-0P, 3-(3-Hydroxyphenyl)-2-methoxypropionic acid methyl ester
477981-20-7P, (2S)-3-[4-(3-Bromopropoxy)phenyl]-2-methoxypropionic acid
ethyl ester 477981-27-4P, (S)-5-(4-Benzyloxybenzyl)-2,2-dimethyl-
[1,3]dioxolan-4-one 477981-33-2P, (S)-5-(4-Hydroxybenzyl)-2,2-dimethyl-
[1,3]dioxolan-4-one 477982-20-0P, 4-[3-(Biphenyl-4-yloxy)propoxy]-2-
fluorobenzaldehyde 477982-21-1P, 3-[4-[3-(Biphenyl-4-yloxy)propoxy]-2-
fluorophenyl]-3-hydroxy-2-methoxypropionic acid methyl ester
477982-22-2P, 3-[4-[3-(Biphenyl-4-yloxy)propoxy]-2-fluorophenyl]-2-
methoxypropionic acid methyl ester 477982-24-4P,
3-(4-Benzyloxyphenyl)-2-(4-chlorophenoxy)propanoic acid methyl ester
477982-25-5P, 2-Phenoxy-3-[4-[3-(4-phenoxyphenoxy)propoxy]phenyl]propanoic
acid methyl ester 477982-27-7P, Methyl 3-hydroxy-2-methoxy-3-[4-
(phenylmethoxy)phenyl]propanoate 477982-28-8P, 3-(4-Hydroxyphenyl)-2-
methoxypropanoic acid 477982-29-9P 477982-30-2P, Ethyl
(2S)-2-methoxy-3-[4-[3-(4-phenoxyphenoxy)propoxy]phenyl]propanoate
477982-37-9P, (2S)-2-Hydroxy-3-[4-[3-(4-phenoxyphenoxy)propoxy]phenyl]prop
ionic acid ethyl ester 477982-38-0P, (2S)-2-Ethoxy-3-[4-[3-(4-

phenoxyphenoxy)propoxy]phenyl]propionic acid ethyl ester 477982-41-5P, (2S)-3-[4-[3-[4-(4-Hydroxybenzoyl)phenoxy]propoxy]phenyl]-2-methoxypropionic acid ethyl ester 477982-42-6P, (2S)-3-[4-[3-[4-[4-[2-(tert-Butyldimethylsilanyloxy)ethoxy]benzoyl]phenoxy]propoxy]phenyl]-2-methoxypropionic acid ethyl ester 477982-45-9P, (2S)-2-Allyloxy-3-(4-benzyloxyphenyl)propionic acid ethyl ester 477982-46-0P, (2S)-3-(4-Hydroxyphenyl)-2-propoxypropionic acid ethyl ester 477982-47-1P, (2S)-3-[4-[3-(4-Phenoxyphenoxy)propoxy]phenyl]-2-propoxypropionic acid ethyl ester 477982-49-3P, (2S)-3-[4-[3-(4-Benzoylphenoxy)propoxy]phenyl]-2-ethoxypropionic acid methyl ester 477982-51-7P, (2S)-3-[4-[3-(4-Benzylphenoxy)propoxy]phenyl]-2-ethoxypropionic acid ethyl ester 477982-53-9P, (2S)-3-(3-Chloro-4-hydroxyphenyl)-2-ethoxypropionic acid ethyl ester 477982-54-0P, (2S)-3-[4-[3-(4-Benzoylphenoxy)propoxy]-3-chlorophenyl]-2-ethoxypropionic acid ethyl ester 477982-56-2P, 3-[4-(3-Hydroxypropoxy)-3-methoxyphenyl]-2-methoxypropionic acid methyl ester 477982-57-3P, (2S)-4'-[3-[2-Methoxy-4-(2-methoxy-2-methoxycarbonylethyl)phenoxy]propoxy]biphenyl-4-carboxylic acid methyl ester 477982-59-5P, 3-[4-(3-Bromopropoxy)-2-methoxy-phenyl]-2-methoxypropionic acid methyl ester 477982-61-9P, (2S)-3-[4-[3-(4'-tert-Butylbiphenyl-4-yloxy)propoxy]-2-methoxyphenyl]-2-methoxypropionic acid methyl ester 477982-64-2P, 4-(2,2,3,3-Tetrafluoropropoxy)1-benzyloxybenzene 477982-65-3P, (2S)-2-Methoxy-3-[4-[3-[4-(2,2,3,3-tetrafluoropropoxy)phenoxy]propoxy]phenyl]propionic acid ethyl ester 477982-68-6P, (2S)-3-[4-[3-(4-Benzyloxyphenoxy)propoxy]phenyl]-2-methoxypropionic acid ethyl ester 477982-69-7P, (2S)-3-[4-[3-(4-Hydroxyphenoxy)propoxy]phenyl]-2-methoxypropionic acid ethyl ester 477982-70-0P, (2S)-2-Methoxy-3-[4-[3-[4-(3-methylbutoxy)phenoxy]propoxy]phenyl]propionic acid ethyl ester 477982-78-8P, (2S)-3-[4-[3-(4-Iodophenoxy)propoxy]phenyl]-2-methoxypropionic acid ethyl ester 477982-79-9P, (2S)-3-[4-[3-[4-(1H-Indol-5-yl)phenoxy]propoxy]phenyl]-2-methoxypropionic acid ethyl ester 477982-84-6P, (2S)-3-[4-[3-(4'-Cyanobiphenyl-4-yloxy)propoxy]phenyl]-2-methoxypropionic acid ethyl ester 477982-86-8P, (2S)-2-Methoxy-3-[4-[3-[4'-(1H-tetrazol-5-yl)biphenyl-4-yloxy]propoxy]phenyl]propionic acid ethyl ester 477982-91-5P, (2S)-2-Methoxy-3-[4-[3-[4-(piperazin-1-yl)phenoxy]propoxy]phenyl]propionic acid ethyl ester 477982-93-7P, (2S)-2-Methoxy-3-[4-[3-[4-(morpholin-4-yl)phenoxy]propoxy]phenyl]propionic acid ethyl ester 477982-95-9P, 3-[4-[3-(Biphenyl-4-yloxy)propoxy]-2-chlorophenyl]-2-hydroxypropionic acid 477982-97-1P, (2S)-3-[4-(2-Bromoethoxy)phenyl]-2-methoxypropionic acid ethyl ester 477983-02-1P, 3-(3-Benzyloxyphenyl)-3-hydroxy-2-methoxypropionic acid methyl ester 477983-03-2P, 3-(3-Benzyloxyphenyl)-2-methoxyacrylic acid methyl ester 477983-04-3P 477983-05-4P, 3-(3-Benzyloxyphenyl)-2-methoxypropionic acid methyl ester 477983-44-1P, 3-[3-(3-Bromopropoxy)phenyl]-2-methoxypropionic acid methyl ester 477983-82-7P, 3-[3-(2-Bromoethoxy)phenyl]-2-methoxypropionic acid methyl ester 477984-10-4P, (2S)-3-(4-Benzyloxyphenyl)-2-propoxypropionic acid ethyl ester 477984-12-6P, 2-Ethoxy-3-(3-hydroxyphenyl)propionic acid methyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of substituted (phenyl)(alkoxy)propanoic acids and analogs as PPAR modulators for treatment of diabetes and related conditions)

IT 57-55-6, Propylene glycol, reactions 69-72-7, 2-Hydroxybenzoic acid, reactions 77-76-9, 2,2-Dimethoxypropane 78-77-3, 1-Bromo-2-methylpropane 79-30-1, Isobutyryl chloride 86-58-8, 8-Quinolineboronic acid 88-69-7, 2-Isopropylphenol 90-05-1, 2-Methoxyphenol 90-15-3, Naphthalen-1-ol 90-43-7, Biphenyl-2-ol 92-69-3, Biphenyl-4-ol 94-18-8, 4-Hydroxybenzoic acid benzyl ester 95-57-8, 2-Chlorophenol

95-65-8, 3,4-Dimethylphenol 98-17-9, 3-Trifluoromethylphenol 98-59-9, p-Toluenesulfonyl chloride **99-07-0**, 3-Dimethylaminophenol 100-02-7, p-Nitrophenol, reactions 100-07-2, 4-Methoxybenzoyl chloride 100-39-0, Benzyl bromide 100-44-7, Benzyl chloride, reactions 101-18-8, 3-Hydroxydiphenylamine 101-53-1, 4-Benzylphenol 103-16-2, 4-Benzyloxyphenol 103-80-0, Phenylacetyl chloride 106-48-9, p-Chlorophenol 106-95-6, Allyl bromide, reactions 107-08-4, Propyl iodide 107-19-7, Propargyl alcohol 108-36-1, 1,3-Dibromobenzene 108-95-2, Phenol, reactions 109-64-8, 1,3-Dibromopropane 110-91-8, Morpholine, reactions 119-36-8, 2-Hydroxybenzoic acid methyl ester 122-01-0, 4-Chlorobenzoyl chloride 122-94-1, 4-Butoxyphenol 123-08-0, 4-Hydroxybenzaldehyde 123-51-3 131-56-6, 2,4-Dihydroxybenzophenone 135-19-3, Naphthalen-2-ol, reactions 142-08-5, Pyridin-2-ol 142-28-9, 1,3-Dichloropropane 150-19-6, 3-Methoxyphenol 321-62-0, 2'-Fluorobiphenyl-4-ol 331-64-6, 2-Fluoro-4-methoxybenzaldehyde 351-54-2, 3-Fluoro-4-methoxybenzaldehyde 371-41-5, 4-Fluorophenol 372-20-3, 3-Fluorophenol 402-45-9, 4-Trifluoromethylphenol 403-43-0, 4-Fluorobenzoyl chloride 485-71-2, (-)-Cinchonidine 504-63-2, 1,3-Propanediol 533-31-3, Benzo[1,3]dioxol-5-ol 540-38-5, p-Iodophenol 557-93-7, 2-Bromopropene 580-16-5, Quinolin-6-ol 580-51-8, Biphenyl-3-ol 585-71-7, (1-Bromoethyl)benzene 599-64-4, 4-Cumylphenol 609-65-4, 2-Chlorobenzoyl chloride 611-20-1, 2-Hydroxybenzonitrile 612-14-6, (2-Hydroxymethylphenyl)methanol 623-50-7, Ethyl glycolate 626-18-6, (3-Hydroxymethylphenyl)methanol 645-45-4, 3-Phenylpropionyl chloride 813-19-4, Bis-tributyltin 817-95-8 831-82-3, 4-Phenoxyphenol 873-62-1, 3-Cyanophenol 874-60-2, 4-Methylbenzoyl chloride 879-18-5, Naphthalene-1-carbonyl chloride 927-68-4, 2-Bromoethyl acetate 927-74-2, 3-Butyn-1-ol 1066-54-2, (Trimethylsilyl)acetylene 1125-78-6, 5,6,7,8-Tetrahydronaphthalen-2-ol 1137-42-4, 4-Benzoylphenol 1198-84-1 1470-94-6, Indan-5-ol 1507-97-7, 1-Cyclopentyl-4-methoxybenzene 1638-22-8, 4-n-Butylphenol 1679-18-1, 4-Chlorophenylboronic acid 1692-15-5, 4-Pyridylboronic acid 1692-25-7, 3-Pyridylboronic acid 1700-30-7, (3-Benzyloxyphenyl)methanol 1700-37-4, 3-Benzyloxybenzaldehyde 1711-05-3, 3-Methoxybenzoyl chloride 1711-06-4, 3-Methylbenzoyl chloride 1711-07-5, 3-Fluorobenzoyl chloride 1765-93-1, 4-Fluorophenylboronic acid 1806-26-4, 4-Octylphenol **1953-54-4**, 1H-Indol-5-ol 1993-03-9, 2-Fluorophenylboronic acid 2243-83-6, Naphthalene-2-carbonyl chloride 2380-84-9, 1H-Indol-7-ol 2426-87-1, 4-Benzyloxy-3-methoxybenzaldehyde 2443-58-5, 9H-Fluoren-2-ol 2491-32-9, Benzyl 4-hydroxyphenyl ketone 2550-36-9, (Bromomethyl)cyclohexane 3174-67-2, 1,3-Pentanediol 3179-63-3 3282-30-2, 2,2-Dimethylpropionyl chloride 3513-81-3, 2-Methylenepropane-1,3-diol 3900-89-8, 2-Chlorophenylboronic acid 4104-33-0 4397-53-9, 4-Benzyloxybenzaldehyde 4541-15-5, 5-Benzyloxypentan-1-ol 4787-77-3, 2-Pyrrolidin-1-ylphenol 5057-98-7, cis-1,2-Cyclopentanediol 5390-04-5, 4-Pentyn-1-ol 5720-07-0, 4-Methoxyphenylboronic acid 6165-68-0, Thiophene-2-boronic acid 6290-49-9, Methyl methoxyacetate 6665-83-4, 6-Hydroxyflavone 6665-86-7, 7-Hydroxyflavone 6949-73-1, 2-Hydroxy-9-fluorenone 7154-85-0, N-(4-Hydroxyphenyl)phthalimide 10041-02-8, 4-(Imidazol-1-yl)phenol 13037-86-0, 4-Heptyloxyphenol 13154-24-0, Triisopropylsilyl chloride 13196-08-2, 3-Phenyl-6-hydroxybenzofuran 17257-71-5, (S)-(-)-α-Methoxy-α-(trifluoromethyl)phenylacetic acid 17299-07-9, (2R,5R)-Hexane-2,5-diol 18162-48-6, tert-Butyldimethylsilyl chloride 19132-06-0 19438-10-9, 3-Hydroxybenzoic acid methyl ester 19812-92-1, 4'-tert-Butylbiphenyl-4-ol 19812-93-2, 4'-Hydroxy-4-biphenylcarbonitrile 21615-34-9, 2-Methoxybenzoyl chloride 23508-35-2, (S)-2-Hydroxy-3-(4-hydroxyphenyl)propionic acid 24347-58-8, (2R,3R)-Butane-2,3-diol

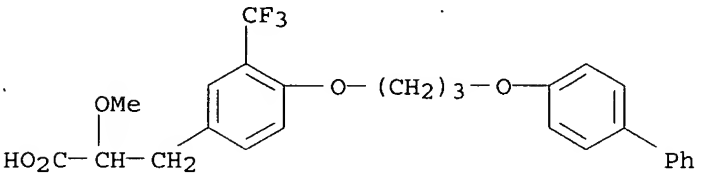
25913-05-7, 4-Fluoro-4'-hydroxybenzophenone 27292-49-5, 3-(4-Morpholino)phenol 34338-96-0, (2S,5S)-Hexane-2,5-diol 37595-74-7, Phenyl triflimide 39634-42-9, 4-(4-Trifluoromethylphenoxy)phenol 40501-41-5, 4'-Hydroxybiphenyl-4-carboxylic acid methyl ester 41351-30-8, 2,4-Dimethoxy-4'-hydroxybenzophenone 41536-44-1, 2-Morpholin-4-ylphenol 42075-32-1, (2R,4R)-Pentanediol 51067-38-0, 4-Phenoxyphenylboronic acid 52222-87-4, (6-Hydroxynaphthalen-2-yl)phenylmethanone 56363-84-9, 2-Chloro-4-hydroxybenzoic 56621-48-8, 1-(4-Hydroxyphenyl)piperazine 59016-93-2, 4-Hydroxymethylphenylboronic acid 60859-24-7, 3-(4-Benzylphenoxy)propyl bromide 63402-63-1, 3-(4-Phenoxyphenoxy)propan-1-ol 63503-60-6, 3-Chlorophenylboronic acid 67914-60-7, 1-Acetyl-4-(4-hydroxyphenyl)piperazine 68867-14-1, 2-Methylbenzothiazol-5-ol 72345-23-4, (2S,4S)-Pentanediol 72569-10-9, 1-(4-Hydroxyphenyl)-2,2-dimethylpropan-1-one 72912-49-3, 2-(2,3,6-Trifluorophenoxy)ethanol 73842-99-6, 3-(tert-Butyldimethylsilanyloxy)propan-1-ol 73852-19-4, 3,5-Bis(trifluoromethyl)phenylboronic acid 74052-89-4, N-(4-Hydroxyphenyl)-2,2-dimethylpropionamide 85459-30-9, Methanesulfonic acid 2,2,3,3-tetrafluoropropyl ester 87184-99-4, 4-(tert-Butyldimethylsilanyloxy)butan-1-ol 87199-16-4, 3-Formylphenylboronic acid 91973-67-0, N-(4-Hydroxyphenyl)nicotinamide 94839-07-3 100124-06-9, 4-Dibenzofuranboronic acid 101969-75-9, 2-Fluoro-4'-hydroxybenzophenone 108357-63-7, [4-(3-Bromopropoxy)phenyl]phenylmethanone 123324-71-0, 4-tert-Butylphenylboronic acid 129742-36-5, 4-tert-Butyldimethylsilanyloxy-2-methoxybenzaldehyde 139301-27-2, 4-Trifluoromethoxybenzeneboronic acid 144104-59-6, 5-Indolylboronic acid 179018-47-4, 2-Fluoro-4-hydroxybenzophenone 179113-90-7, 3-Trifluoromethoxybenzeneboronic acid 222555-06-8, (2S)-2-Ethoxy-3-(4-hydroxyphenyl)propionic acid ethyl ester 253785-18-1, [4-(3-Hydroxypropoxy)phenyl]phenylmethanone 325793-74-6, (2S)-2-Ethoxy-3-(4-hydroxyphenyl)propionic acid methyl ester 438526-21-7 477979-20-7, (S)-2-Methoxy-3-(4-hydroxyphenyl)propionic acid ethyl ester 477979-36-5, 6-Hydroxy-3-(4-fluorophenyl)benzofuran 477979-46-7, (2S)-3-[4-(5-Hydroxypent-1-ynyl)phenyl]-2-methoxypropionic acid 477979-79-6, (2S)-3-[4-(4-Hydroxybut-1-ynyl)phenyl]-2-methoxypropionic acid ethyl ester 477979-81-0, (2S)-3-(4-Iodophenyl)-2-methoxypropionic acid ethyl ester 477980-31-7 477980-43-1, (2S)-3-(4-Hydroxyphenyl)-2-methoxypropionic acid 477980-43-1D, (2S)-3-(4-Hydroxyphenyl)-2-methoxypropionic acid, resin bound 477980-45-3D, (2S)-3-[4-(3-Hydroxypropoxy)phenyl]-2-methoxypropionic acid, resin bound 477980-74-8D, 3-[4-(3-Hydroxypropoxy)-3-methoxyphenyl]-2-methoxypropionic acid, resin bound 477981-12-7, (2S)-3-[4-[3-[4-(4-Fluorobenzoyl)phenoxy]propoxy]phenyl]-2-methoxypropionic acid ethyl ester 477981-18-3, (2S)-3-[4-(3-Hydroxypropoxy)phenyl]-2-methoxypropionic acid ethyl ester 477981-36-5, 3-[4-(3-Bromopropoxy)-3-methoxyphenyl]-2-methoxypropionic acid 477981-42-3, 4-Dibenzofuran-3-ylphenol 477981-45-6, (2S)-3-[4-(4-Bromobutoxy)phenyl]-2-methoxypropionic acid ethyl ester 477981-56-9 477981-64-9, 3-(2-Chloro-4-hydroxyphenyl)-2-methoxypropionic acid ethyl ester 477981-71-8, 4-Dibenzothiophen-4-ylphenol 477982-32-4, (2S)-2-Methoxy-3-[4-[2-(4-phenoxyphenoxy)propoxy]phenyl]propionic acid 477982-33-5, 3-[4-[2-Methylene-3-(4-phenoxyphenoxy)propoxy]phenyl]propionic acid 477982-60-8, 3-(4-Hydroxy-2-methoxyphenyl)-2-methoxypropionic acid methyl ester 477982-66-4, 3-[4-(3-Bromopropoxy)phenyl]-2-methoxypropionic acid ethyl ester 477984-00-2 477984-14-8, (S)-3-[4-[3-(4'-Bromobiphenyl-4-yloxy)propoxy]phenyl]-2-methoxypropionic acid

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of substituted (phenyl)(alkoxy)propanoic acids and analogs as PPAR modulators for treatment of diabetes and related conditions)

IT **477980-89-5P**, 3-[4-[3-(Biphenyl-4-yloxy)propoxy]-3-trifluoromethylphenyl]-2-methoxypropionic acid
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(PPAR modulator; preparation of substituted (phenyl)(alkoxy)propanoic acids and analogs as PPAR modulators for treatment of diabetes and related conditions)

RN 477980-89-5 HCAPLUS

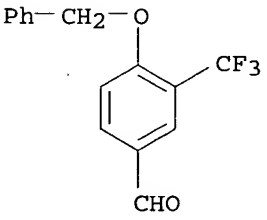
CN Benzenepropanoic acid, 4-[3-([1,1'-biphenyl]-4-yloxy)propoxy]-α-methoxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



IT **477980-90-8P**, 4-Benzyloxy-3-trifluoromethylbenzaldehyde
477980-92-0P, 3-[4-[3-(Biphenyl-4-yloxy)propoxy]-3-trifluoromethylphenyl]-2-methoxyacrylic acid methyl ester
477980-93-1P, 3-[4-[3-(Biphenyl-4-yloxy)propoxy]-3-trifluoromethylphenyl]-2-methoxyacrylic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of substituted (phenyl)(alkoxy)propanoic acids and analogs as PPAR modulators for treatment of diabetes and related conditions)

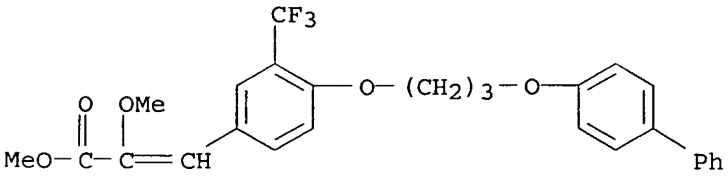
RN 477980-90-8 HCAPLUS

CN Benzaldehyde, 4-(phenylmethoxy)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

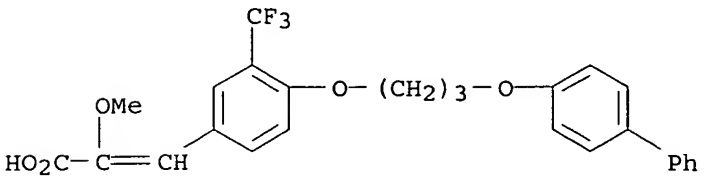


RN 477980-92-0 HCAPLUS

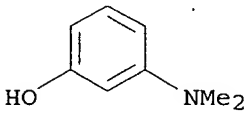
CN 2-Propenoic acid, 3-[4-[3-([1,1'-biphenyl]-4-yloxy)propoxy]-3-(trifluoromethyl)phenyl]-2-methoxy-, methyl ester (9CI) (CA INDEX NAME)



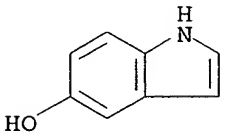
RN 477980-93-1 HCAPLUS
CN 2-Propenoic acid, 3-[4-[3-([1,1'-biphenyl]-4-yloxy)propoxy]-3-(trifluoromethyl)phenyl]-2-methoxy- (9CI) (CA INDEX NAME)



IT **99-07-0**, 3-Dimethylaminophenol **1953-54-4**, 1H-Indol-5-ol
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of substituted (phenyl)(alkoxy)propanoic acids and analogs as PPAR modulators for treatment of diabetes and related conditions)
RN 99-07-0 HCAPLUS
CN Phenol, 3-(dimethylamino)- (9CI) (CA INDEX NAME)



RN 1953-54-4 HCAPLUS
CN 1H-Indol-5-ol (9CI) (CA INDEX NAME)



L33 ANSWER 9 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:655599 HCAPLUS
DOCUMENT NUMBER: 137:337755
TITLE: Synthesis of New Molecules Containing Head, Spacer, and Label Moieties
AUTHOR(S): Khatyr, Abderrahim; Maas, Huub; Calzaferri, Gion
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of Bern, Bern, CH-3012, Switz.
SOURCE: Journal of Organic Chemistry (2002), 67(19), 6705-6710
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB We describe the synthesis and characterization of novel stopcock mols. containing a head with precise shape, spacer, and label moieties. The protocol is based on a Pd(0)-catalyzed cross-coupling reaction between ethynylphenyl/bromide to obtain a rigid head followed by the attachment of a flexible spacer possessing two reactive functional groups on the termini. The final step consists of forming a covalent bond between spacer and label. In addition, monosubstituted soluble labels were synthesized in good yields. Examples of the products are I and II.

CC 27-14 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 28, 41

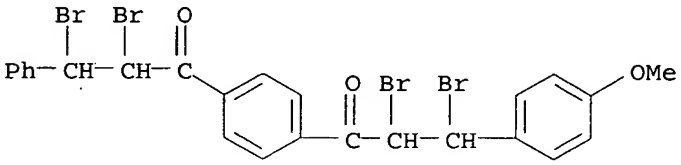
IT **Dyes**
(preparation of soluble dyes)

IT 473933-46-9P 473933-48-1P **473933-50-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of soluble dyes)

IT **473933-50-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of soluble dyes)

RN 473933-50-5 HCAPLUS

CN 1-Propanone, 2,3-dibromo-1-[4-[2,3-dibromo-3-(4-methoxyphenyl)-1-oxopropyl]phenyl]-3-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 10 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:153776 HCAPLUS
DOCUMENT NUMBER: 136:365624
TITLE: Design and Synthesis of Class-Selective Activity Probes for Protein Tyrosine Phosphatases
AUTHOR(S): Lo, Lee-Chiang; Pang, Te-Ling; Kuo, Chi-Hsien; Chiang, Ying-Ling; Wang, Hsin-Yi; Lin, Jing-Jer
CORPORATE SOURCE: Department of Chemistry, National Taiwan University, Taipei, 106, Taiwan
SOURCE: Journal of Proteome Research (2002), 1(1), 35-40
CODEN: JPROBS; ISSN: 1535-3893
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

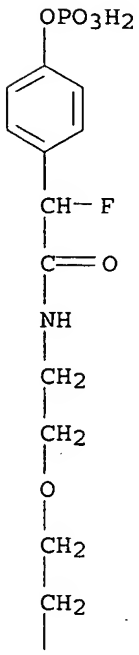
AB Two mechanism-based activity probes, adopting a cassette-like design, for protein tyrosine phosphatases (PTPs) were synthesized. Both probes carry a phosphate group that serves as the recognition head for the target PTPs but differ in their reporter groups; probe LCL-1 uses a dansyl fluorophore, while LCL-2 has a biotin reporter group. LCL-1 and LCL-2 are specifically activated by phosphatase, leading to its covalent labeling, as exemplified with PTP-1B. However, they show no activation with other classes of hydrolases, including trypsin and β-galactosidase. LCL-1 and LCL-2 thus represent the first example of class-selective probes for

phosphatases.
CC 7-3 (Enzymes)
IT **423756-10-9P 423756-12-1P**
RL: BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(protein tyrosine phosphatase can be labeled by class-selective activity probes LCL-1 and LCL-2)
IT 605-65-2, Dansyl chloride **35013-72-0**, (N-Hydroxysuccinimidyl)biotin **252259-78-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(protein tyrosine phosphatase can be labeled by class-selective activity probes LCL-1 and LCL-2)
IT **423756-07-4P 423756-08-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(protein tyrosine phosphatase can be labeled by class-selective activity probes LCL-1 and LCL-2)
IT **423756-10-9P 423756-12-1P**
RL: BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(protein tyrosine phosphatase can be labeled by class-selective activity probes LCL-1 and LCL-2)
RN 423756-10-9 HCAPLUS
CN Benzeneacetamide, N-[2-[2-[2-[[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]amino]ethoxy]ethoxy]ethyl]-α-fluoro-4-(phosphonooxy)-, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 423756-09-6
CMF C26 H33 F N3 O9 P S

PAGE 1-A



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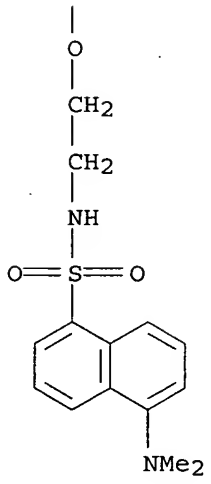
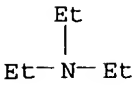


CM 2

CRN 121-44-8
CMF C6 H15 N



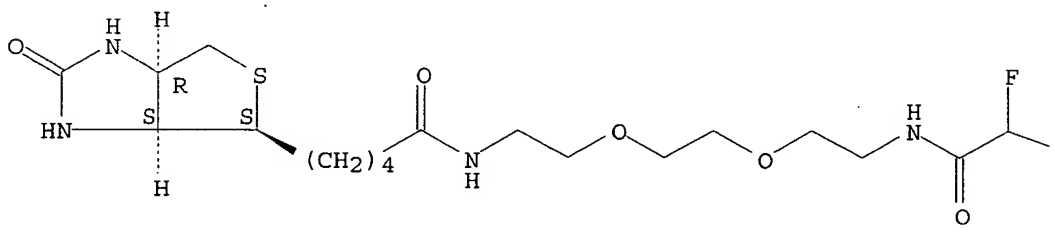
RN 423756-12-1 HCAPLUS
CN 1H-Thieno[3,4-d]imidazole-4-pentanamide, N-[2-[2-[2-[[fluoro[4-(phosphonooxy)phenyl]acetyl]amino]ethoxy]ethoxy]ethyl]hexahydro-2-oxo-, (3aS,4S,6aR)-, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 423756-11-0
CMF C24 H36 F N4 O9 P S

Absolute stereochemistry.

PAGE 1-A



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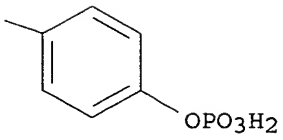

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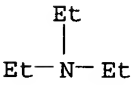
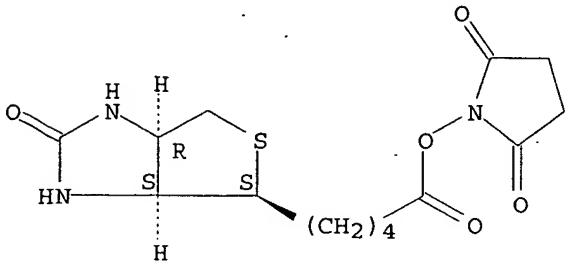


IT **35013-72-0**, (N-Hydroxysuccinimidyl)biotin **252259-78-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(protein tyrosine phosphatase can be labeled by class-selective activity probes LCL-1 and LCL-2)

RN 35013-72-0 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[5-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-1-oxopentyl]oxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 252259-78-2 HCAPLUS
CN Phosphoric acid, 4-[2-[[2-[2-(2-aminoethoxy)ethoxy]ethyl]amino]-1-fluoro-2-oxoethyl]phenyl di-2-propenyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 252259-77-1
CMF C20 H30 F N2 O7 P

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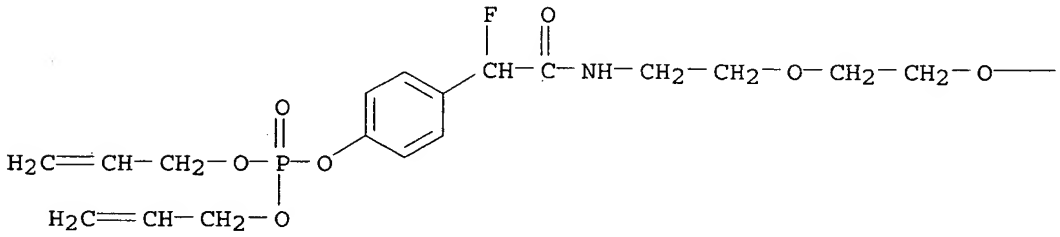
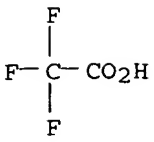


PAGE 1-B

CM 2

CRN 76-05-1
CMF C2 H F3 O2



IT **423756-07-4P 423756-08-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(protein tyrosine phosphatase can be labeled by class-selective activity probes LCL-1 and LCL-2)

RN 423756-07-4 HCAPLUS

CN Phosphoric acid, 4-[2-[[2-[2-[2-[[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]amino]ethoxy]ethoxy]ethyl]amino]-1-fluoro-2-oxoethyl]phenyl di-2-propenyl ester (9CI) (CA INDEX NAME)

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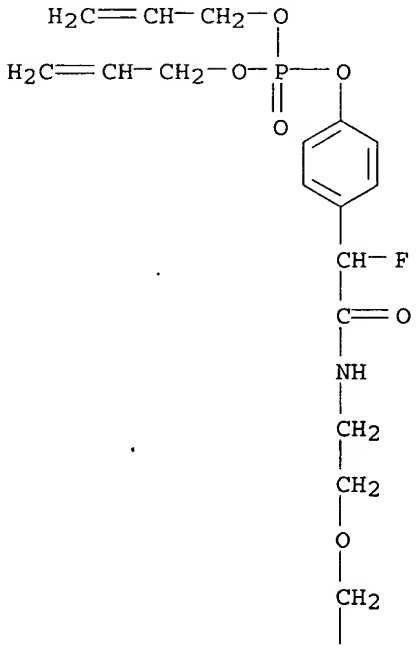

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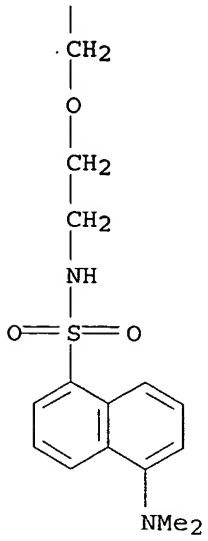
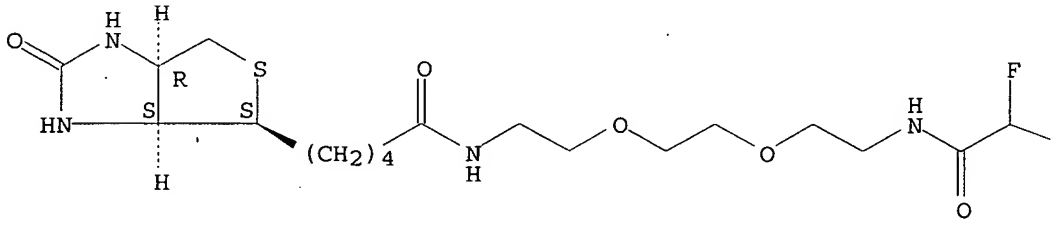


RN 423756-08-5 HCAPLUS
CN Phosphoric acid, 4-[1-fluoro-17-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-2,13-dioxo-6,9-dioxa-3,12-diazaheptadec-1-yl]phenyl di-2-propenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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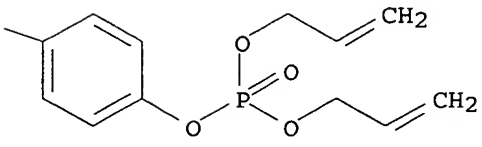

REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 11 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:833867 HCAPLUS
DOCUMENT NUMBER: 135:357774

TITLE: Preparation of phthalic acid diamides as agricultural and horticultural insecticides

INVENTOR(S): Tohnishi, Masanori; Nakao, Hayami; Kohno, Eiji; Nishida, Tateki; Furuya, Takashi; Shimizu, Toshiaki; Seo, Akira; Sakata, Kazuyuki; Fujioka, Shinsuke; Kanno, Hideo

PATENT ASSIGNEE(S): Nihon Nohyaku Co., Ltd., Japan

SOURCE: U.S. Pat. Appl. Publ., 114 pp., Cont.-in-part of U.S. Ser. No. 198,391, abandoned.
CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2001041814	A1	20011115	US 1999-250261	19990216
US 6362369	B2	20020326		
US 2003055287	A1	20030320	US 2002-35132	20020104
US 6559341	B2	20030506		

PRIORITY APPLN. INFO.:

JP 1997-339393	A	19971125
JP 1998-51351	A	19980217
US 1998-198391	B2	19981124
US 1999-250261	A3	19990216

OTHER SOURCE(S): MARPAT 135:357774

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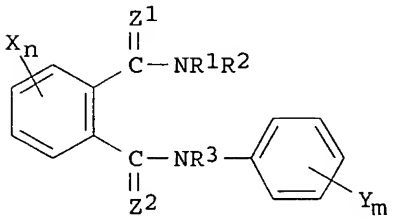

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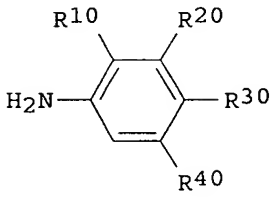

II

AB The title compds. [I; R1-R3 = H, CN, cycloalkyl, etc.; X = H, CN, NO2, etc.; n = 1-4; Y = H, halo, CN, etc.; m = 1-5; Z1, Z2 = O, S] which show excellent activities for controlling injurious insects, were prepared Thus, reaction of 3-nitro-2-ethoxycarbonylbenzoyl chloride with 4-chloro-2-methylaniline in the presence of Et3N in THF followed by treatment of the resulting Et 6-nitro-N-(4-chloro-2-methylphenyl)phthalamate with isopropylamine in dioxane afforded I [R1 = iso-Pr; R2 = R3 = H; X = 3-NO2; Y = 2-Me-4-Cl; Z1 = Z2 = O] which showed excellent insecticidal effect (100% mortality) against diamondback moth and common cutworm. The fluorine-containing anilines II [R10 = halo, alkyl, alkoxy, CF3; R20, R30, R40 = H or perfluoroalkyl; provided that at least one of R20-R40 is not H atom, and that R30 is neither a pentafluoroethyl nor a n-heptafluoropentyl when R10 = F and each of R20 and R40 = H], useful as a starting material for said phthalic acid diamides were also prepared

IC ICM C07C233-00

NCL 564156000

CC 25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 5

IT 16497-37-3P 16497-38-4P 226958-87-8P 226958-88-9P 226958-89-0P
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RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of phthalic acid diamides as agricultural and horticultural insecticides)

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226963-70-8P 226963-71-9P 226963-72-0P 226963-73-1P 226963-74-2P
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226963-80-0P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of phthalic acid diamides as agricultural and horticultural insecticides)

IT 226963-81-1P 226963-82-2P 226963-83-3P **226963-84-4P**
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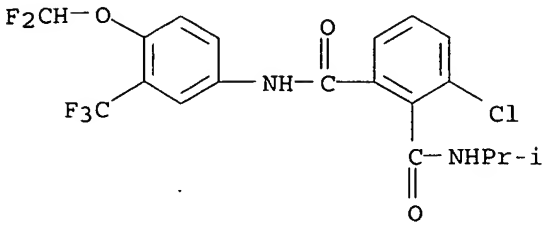
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of phthalic acid diamides as agricultural and horticultural insecticides)

IT **95-69-2**, 4-Chloro-2-methylaniline 117-21-5, 3-Chlorophthalic anhydride 461-82-5, 4-Trifluoromethoxyaniline 641-70-3 677-69-0, 2-Iodoheptafluoropropane 2253-73-8, Isopropyl isothiocyanate 13194-68-8 28394-52-7 28418-88-4, 3-Iodophthalic anhydride 39211-40-0 39211-57-9 42016-93-3, 2-Chloro-4-iodoaniline 52415-00-6 226979-97-1 226979-98-2 238098-39-0 372193-51-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of phthalic acid diamides as agricultural and horticultural insecticides)

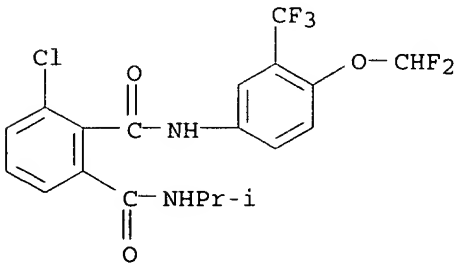
IT **226960-70-9P 226961-60-0P 226963-22-0P**
226963-84-4P 226966-20-7P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of phthalic acid diamides as agricultural and horticultural insecticides)

RN 226960-70-9 HCAPLUS
CN 1,2-Benzenedicarboxamide, 3-chloro-N1-[4-(difluoromethoxy)-3-

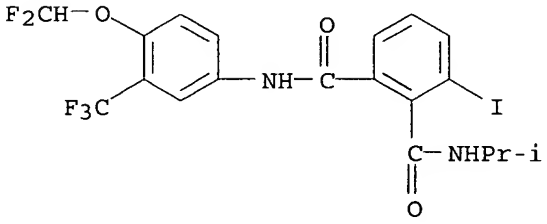
(trifluoromethyl)phenyl]-N2-(1-methylethyl)- (9CI) (CA INDEX NAME)



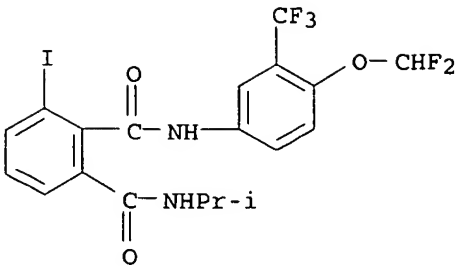
RN 226961-60-0 HCAPLUS
CN 1,2-Benzenedicarboxamide, 3-chloro-N2-[4-(difluoromethoxy)-3-(trifluoromethyl)phenyl]-N1-(1-methylethyl)- (9CI) (CA INDEX NAME)



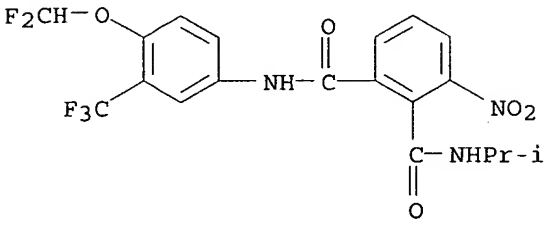
RN 226963-22-0 HCAPLUS
CN 1,2-Benzenedicarboxamide, N1-[4-(difluoromethoxy)-3-(trifluoromethyl)phenyl]-3-iodo-N2-(1-methylethyl)- (9CI) (CA INDEX NAME)



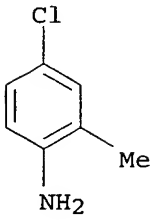
RN 226963-84-4 HCAPLUS
CN 1,2-Benzenedicarboxamide, N2-[4-(difluoromethoxy)-3-(trifluoromethyl)phenyl]-3-iodo-N1-(1-methylethyl)- (9CI) (CA INDEX NAME)



RN 226966-20-7 HCAPLUS
CN 1,2-Benzenedicarboxamide, N1-[4-(difluoromethoxy)-3-(trifluoromethyl)phenyl]-N2-(1-methylethyl)-3-nitro- (9CI) (CA INDEX NAME)



IT **95-69-2**, 4-Chloro-2-methylaniline
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of phthalic acid diamides as agricultural and horticultural insecticides)
RN 95-69-2 HCAPLUS
CN Benzenamine, 4-chloro-2-methyl- (9CI) (CA INDEX NAME)



L33 ANSWER 12 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:152525 HCAPLUS
DOCUMENT NUMBER: 134:212695
TITLE: Drug conjugates comprising vector-linker-pharmacophore and methods of designing the same
INVENTOR(S): Brenner, Sydney; Goelet, Philip; Stackhouse, Joseph; Millward, Steven W.
PATENT ASSIGNEE(S): USA
SOURCE: PCT Int. Appl., 196 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001013958	A2	20010301	WO 2000-US23593	20000828
WO 2001013958	A3	20020131		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2382202	AA	20010301	CA 2000-2382202	20000828
EP 1212096	A2	20020612	EP 2000-959512	20000828
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003507439	T2	20030225	JP 2001-518093	20000828
PRIORITY APPLN. INFO.:			US 1999-150765P	P 19990826
			US 1999-150894P	P 19990826
			US 2000-184411P	P 20000223
			US 2000-184412P	P 20000223
			WO 2000-US23593	W 20000828

AB The invention relates to drug conjugates and methods of their design. One embodiment of the invention is directed to a method of designing vector-linker-pharmacophore (VLP) conjugates that is generally applicable to a wide variety of vectors, linkers, and pharmacophores. The invention also encompasses a method of improving the delivery of a pharmacophore to a patient, as well as a method of improving the therapeutic efficacy of a pharmacophore and a method of decreasing the toxicity of a pharmacophore. A method of increasing the concentration of a pharmacophore in a cell is further encompassed by the invention. Preparation of many VLP conjugates including conjugates of kirromycin-3-nitro-4-hydrazidophenylthioethanol-tetracycline derivative, are disclosed.

IC ICM A61K047-48

CC 63-5 (Pharmaceuticals)
Section cross-reference(s): 28

IT **58-85-5DP**, Biotin, conjugate with penicillin derivs.
58-85-5DP, Biotin, conjugates 60-54-8DP, Tetracycline, conjugates 525-97-3DP, Penicillin a, derivs., conjugate with biotin 738-70-5DP, Trimethoprim, conjugates 738-70-5DP, Trimethoprim, reaction with kirromycin conjugates 1406-05-9DP, Penicillin, conjugates 11076-17-8DP, Sordarin, conjugates with antibiotics 86386-73-4DP, Fluconazole, conjugates 328401-25-8P 328401-69-0DP, reaction with tetracycline and trimethoprim derivs.
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug conjugates comprising vector-linker-pharmacophore and methods of designing same)

IT 50-00-0, Formaldehyde, reactions 60-23-1, 2-Mercaptoethylamine 60-54-8D, Tetracycline, reaction with kirromycin conjugates 64-17-5, Ethanol, reactions 64-18-6, Formic acid, reactions 97-51-8, 5-Nitrosalicylaldehyde 100-39-0, Benzyl bromide 103-84-4, Acetylaniline 108-24-7, Acetic anhydride 109-64-8, 1,3 DiBromopropane

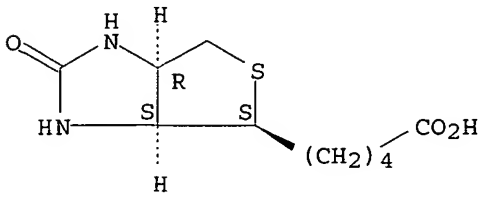
111-30-8, Glutardialdehyde 124-40-3, Dimethylamine, reactions 124-41-4, Sodium methoxide 124-63-0, Methylsulfonyl chloride 142-28-9, 1,3 Dichloropropane 156-81-0, 2,4 Diaminopyrimidine 302-01-2, Hydrazine, reactions 530-62-1 540-88-5, Tert-Butylacetate 551-16-6, 6-Aminopenicillanic acid .598-21-0, BROMOACETYL BROMIDE 601-89-8, 2-Nitroresorcinol 605-65-2, Dansyl chloride 624-84-0, Formyl hydrazine 627-31-6 928-01-8, Maleamide 1003-10-7, γ-Thiobutyrolactone 1197-55-3, 4-Aminophenylacetic acid 1313-82-2, Sodium sulfide, reactions 2393-24-0 2950-43-8, Hydroxylamine-O-sulfonic acid 3483-12-3, Dithiothreitol 3963-95-9, Methacycline hydrochloride 4163-60-4 4829-04-3, 1,3-Dithiolane 5414-21-1, 5-Bromovaleronitrile 5470-11-1, Hydroxylamine hydrochloride 6258-60-2, 4-Methoxybenzylmercaptan 6539-14-6, Traut's reagent 6625-20-3, 6-Demethyl 6 deoxytetracycline hydrochloride 7631-99-4, Sodium nitrate, reactions 7664-41-7, Ammonia, reactions 7681-49-4, Sodium fluoride, reactions 7697-37-2, Nitric acid, reactions 7790-28-5, Sodium periodate 7791-25-5, Sulfonyl chloride 10028-15-6, Ozone, reactions 10035-10-6, Hydrobromic acid, reactions 10592-13-9, Doxycycline hydrochloride 13154-24-0, Triisopropylsilyl chloride 16940-66-2, Sodium borohydride 21908-53-2, Mercuric oxide 22542-53-6 23361-78-6 25155-26-4, Dimethoxyphenol 25895-60-7, Sodium cyanoborohydride 38078-09-0, Diethylaminosulfur trifluoride 41661-47-6, 4-Piperidone 50935-71-2, Kirromycin 53152-67-3 69468-17-3, Diaminobutane 72040-63-2 84030-21-7 93285-75-7 **109276-34-8** 134759-23-2 205584-10-7 328400-58-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(drug conjugates comprising vector-linker-pharmacophore and methods of designing same)

IT 104-10-9P 107-68-6P, N-Methyltaurine 501-53-1P, Carbobenzyloxy chloride 1007-54-1P 3163-15-3P, 2-Aminoresorcinol 5063-96-7P 6066-83-7P, 5-Aminovaleronitrile 15896-61-4P 17385-61-4P 19285-38-2P 21253-57-6P 21253-58-7P 21822-24-2P 52648-14-3P, 1-N-Desmethylgoldinamine 73164-56-4P 74219-55-9P 86386-77-8P 116435-82-6P 120793-45-5P 143429-10-1P 155834-18-7P 161321-16-0P 161321-34-2P 188434-24-4P **188434-25-5P 188434-26-6P** 328400-43-7P 328400-46-0P 328400-48-2P 328400-50-6P 328400-52-8P 328400-54-0P 328400-56-2P 328400-60-8P 328400-62-0P 328400-64-2P 328400-66-4P 328400-68-6P 328400-71-1P 328400-73-3P 328400-75-5P 328400-77-7P 328400-79-9P 328400-81-3P 328400-83-5P 328400-87-9P 328400-89-1P 328400-91-5P 328400-93-7P 328400-95-9P 328400-98-2P 328401-02-1P 328401-08-7P 328401-09-8P 328401-10-1P 328401-11-2P 328401-12-3P 328401-13-4P 328401-14-5P 328401-15-6P 328401-16-7P **328401-17-8P 328401-18-9P 328401-19-0P** 328401-20-3P 328401-21-4P 328401-22-5P 328401-23-6P 328401-24-7P 328401-26-9P 328401-27-0P 328401-28-1P 328401-29-2P 328401-30-5P 328401-31-6P 328401-32-7P 328401-33-8P 328401-34-9P 328401-35-0P 328401-36-1P 328401-37-2P 328401-38-3P 328401-39-4P 328401-40-7P 328401-41-8P 328401-42-9P 328401-43-0P 328401-44-1P 328401-45-2P 328401-46-3P 328401-47-4P 328401-48-5P 328401-49-6P 328401-50-9P 328401-51-0P 328401-53-2P 328401-54-3P 328401-55-4P 328401-57-6P 328401-59-8P 328401-61-2P 328401-63-4P 328401-64-5P 328401-66-7P 328401-68-9P 328401-69-0DP, derivs. 328401-71-4P 328401-72-5P 328401-73-6P 328401-74-7P 328401-75-8P 328401-76-9P 328401-77-0P 328899-82-7P, Goldinonic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(drug conjugates comprising vector-linker-pharmacophore and methods of designing same)

IT **58-85-5DP**, Biotin, conjugate with penicillin derivs.
RL: BAC (Biological activity or effector, except adverse); BSU (Biological

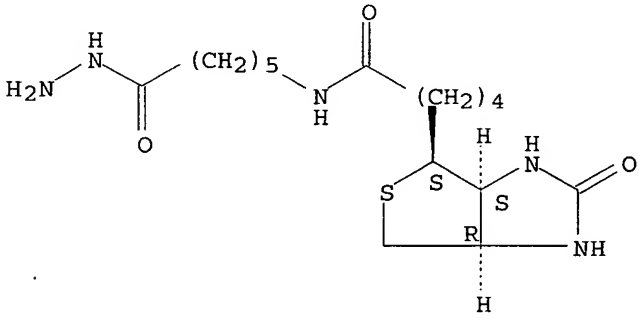
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug conjugates comprising vector-linker-pharmacophore and methods of designing same)
RN 58-85-5 HCAPLUS
CN 1H-Thieno[3,4-d]imidazole-4-pentanoic acid, hexahydro-2-oxo-, (3aS,4S,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



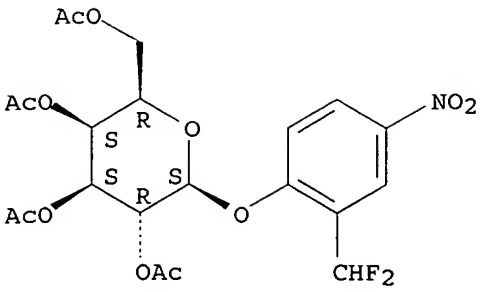
IT **109276-34-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(drug conjugates comprising vector-linker-pharmacophore and methods of designing same)
RN 109276-34-8 HCAPLUS
CN Hexanoic acid, 6-[[5-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-1-oxopentyl]amino]-, hydrazide (9CI) (CA INDEX NAME)

Absolute stereochemistry.



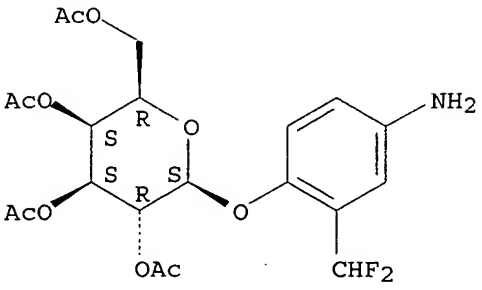
IT **188434-25-5P 188434-26-6P 328401-17-8P 328401-18-9P 328401-19-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(drug conjugates comprising vector-linker-pharmacophore and methods of designing same)
RN 188434-25-5 HCAPLUS
CN β-D-Galactopyranoside, 2-(difluoromethyl)-4-nitrophenyl, 2,3,4,6-tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



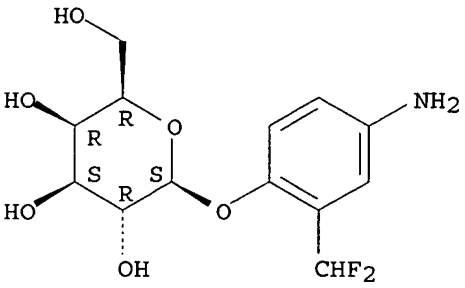
RN 188434-26-6 HCAPLUS
CN β-D-Galactopyranoside, 4-amino-2-(difluoromethyl)phenyl, 2,3,4,6-tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



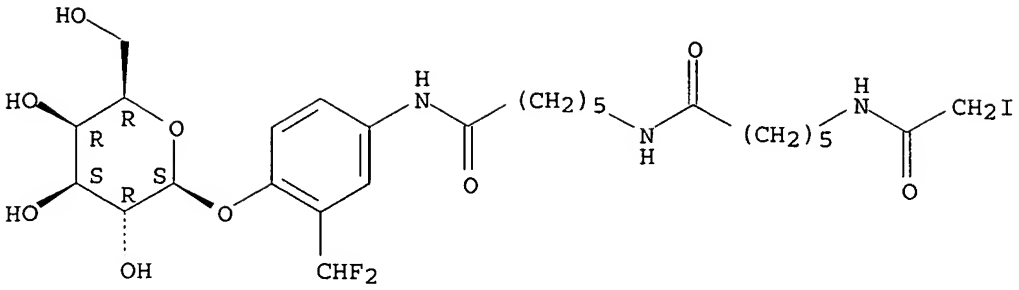
RN 328401-17-8 HCAPLUS
CN β-D-Galactopyranoside, 4-amino-2-(difluoromethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 328401-18-9 HCAPLUS
CN Hexanamide, N-[6-[[3-(difluoromethyl)-4-(β-D-galactopyranosyloxy)phenyl]amino]-6-oxohexyl]-6-[(iodoacetyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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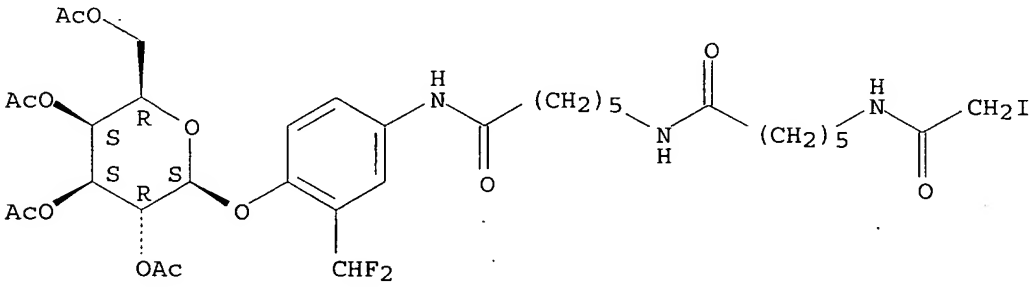
Absolute stereochemistry.



L33 ANSWER 13 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:573671 HCAPLUS
DOCUMENT NUMBER: 133:177183
TITLE: Preparation of quinazoline derivatives as angiogenesis inhibitors
INVENTOR(S): Hennequin, Laurent Francois Andre; Ple, Patrick; Stokes, Elaine Sophie Elizabeth; Mckerrecher, Darren
PATENT ASSIGNEE(S): Astrazeneca UK Limited, UK; Zeneca-Pharma S.A.
SOURCE: PCT Int. Appl., 346 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000047212	A1	20000817	WO 2000-GB373	20000208

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
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CA 2362715	AA	20000817	CA 2000-2362715		20000208
EP 1154774	A1	20011121	EP 2000-902730		20000208
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EE 200100409	A	20021216	EE 2001-409		20000208
AU 763618	B2	20030731	AU 2000-24475		20000208
NZ 513204	A	20040430	NZ 2000-513204		20000208
ZA 2001006340	A	20021101	ZA 2001-6340		20010801
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OTHER SOURCE(S): MARPAT 133:177183

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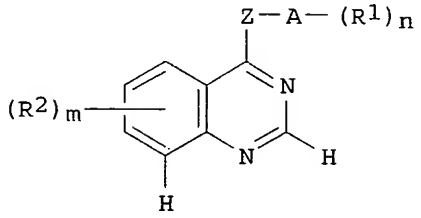

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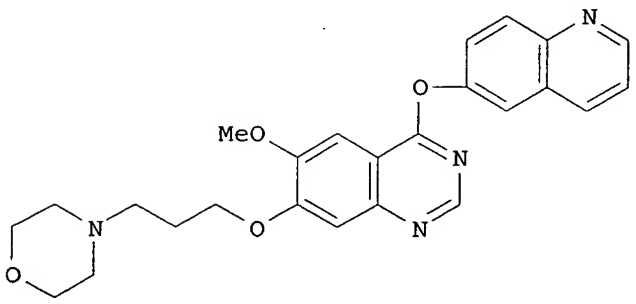


II

AB The title compds. (I) [wherein A = an 8-, 9-, 10-, 12- or 13-membered bicyclic or tricyclic ring optionally containing 1-3 O, N, and/or S heteroatoms; Z = O, NH, S, CH2, or a bond; n = 0-5; m = 0-3; R2 = H, OH, halo, CN, NO2, CF3, alkyl(sulfanyl), alkoxy, NR3N4, or R5X1; R3 and R4 = independently H or alkyl; X1 = a bond, O, CH2, OC(O), CO, S, SO, SO2, NR6CO, CONR7, SO2R8, NR9SO2, or NR10; R5 = H or (un)substituted alkyl, alkenyl, alkynyl, or heterocyclyl, etc.; R6-R10 = independently H or (alkoxy)alkyl] were prepared for use in the production of an antiangiogenic and/or vascular permeability reducing effect in warm-blooded animals. For instance, II was synthesized in a 9-step sequence starting with the cyclization of 2-amino-4-benzyloxy-5-methoxybenzamide using Gold's reagent in dioxane to form 7-benzyloxy-6-methoxy-3,4-dihydroquinazolin-4-one (84%). I and the pharmaceutically acceptable salts thereof inhibit the effects of VEGF, a property of value in the treatment of a number of disease states including cancer and rheumatoid arthritis (no data).

IC ICM A61K031-505
ICS C07D401-14; C07D413-14; C07D417-12; C07D405-12; C07D401-12

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1

IT 622-26-4P, 2-(Piperidin-4-yl)-1-ethanol 2058-49-3P, 3-(Methylsulfonyl)-1-propanol 2380-83-8P, 5-Hydroxy-6-methoxyindole 3373-00-0P, 6-Hydroxy-1,2,3,4-tetrahydroquinoline 3603-45-0P, 2-(2-Morpholinoethoxy)ethanol 4332-48-3P, Ethyl 3-(1H-1,2,3-triazol-1-yl)propanoate 4441-30-9P, 4-(3-Hydroxypropyl)morpholine 4887-81-4P, 5-Methoxy-2-methylbenzimidazole 5317-33-9P, 1-(3-Hydroxypropyl)-4-methylpiperazine 5318-27-4P, 6-Aminoindole 5464-12-0P, 4-(2-Hydroxyethyl)-1-methylpiperazine 7357-67-7P, 1-Chloro-3-morpholinopropane 7556-97-0P, 7-Hydroxyquinazoline 10312-83-1P, Methoxyacetaldehyde 13280-07-4P, 4-Chlorobut-2-yn-1-ol 13314-85-7P, 5-Hydroxy-2-methylindole 13523-92-7P, 5-Hydroxy-1-methylindole 13790-39-1P, 4-Chloro-6,7-dimethoxyquinazoline 13794-72-4P, 6,7-Dimethoxy-3,4-dihydroquinazolin-4-one 14597-28-5P, 4-(Pyrrolidin-1-yl)but-2-yn-1-ol 36729-22-3P, 2,3-Dimethyl-5-hydroxyindole **39062-69-6P**, 2-Benzyloxy-5-nitrotrifluoromethylbenzene 41292-66-4P, 5-Hydroxy-2-methylbenzimidazole 56058-21-0P, 1-(3-Hydroxypropyl)pyrrolidin-2,5-dione 63762-83-4P, 6-Fluoro-5-methoxyindole 71082-46-7P, 3-Ethoxycarbonyl-7-methoxyquinoline 71083-05-1P, Ethyl 7-methoxy-4-oxo-1,4-dihydroquinoline-3-carboxylate 71083-35-7P, 3-Carbamoyl-7-methoxyquinoline 71083-49-3P, 3-Cyano-7-methoxyquinoline 76243-24-8P, 2-Fluoro-4-nitrobenzyloxybenzene 77156-85-5P, 4-Chloro-3-ethoxycarbonyl-7-methoxyquinoline 84497-70-1P, 3-(1H-1,2,4-Triazol-1-yl)propan-1-ol 84497-72-3P, 3-(5-Methyl-[1,2,4]triazol-1-yl)propan-1-ol 89151-44-0P, 4-(2-Hydroxyethyl)-1-(tert-butoxycarbonyl)piperidine 89151-45-1P, 4-[2-(4-Methylphenylsulfonyloxy)ethyl]-1-tert-butoxycarbonylpiperidine 90858-86-9P, 4-Bromo-5-methoxyindole 92622-97-4P, 4-Bromo-5-methoxyindole-2-carboxylic acid 121247-16-3P, 3-Acetylmethyl-1,2-difluoro-4-nitrobenzene 123387-51-9P, 4,4-(Ethylenedioxy)-1-tert-butoxycarbonylpiperidine 123855-51-6P, 4-Hydroxymethyl-1-tert-butoxycarbonylpiperidine 135531-89-4P, 5-Hydroxy-4-nitroindole 135531-92-9P, 5-Methoxy-4-nitroindole 135716-09-5P, Ethyl 1-tert-butyloxycarbonyl-4-piperidinecarboxylate 162364-72-9P, 7-Benzyloxy-4-chloro-6-methoxyquinazoline 163210-40-0P, 2-[[1-(tert-Butoxycarbonyl)piperidin-4-yl]oxy]ethanol 174734-34-0P, 5-Methoxy-2-trifluoromethylindole 179688-01-8P, 7-Benzyloxy-6-methoxy-3,4-dihydroquinazolin-4-one 181950-57-2P, 4-Chloro-7-hydroxyquinoline 193001-44-4P, 7-Benzyloxy-4-chloro-6-methoxyquinazoline hydrochloride 193001-55-7P, 7-Benzyloxy-6-methoxy-4-phenoxyquinazoline 193001-56-8P, 7-Hydroxy-6-methoxy-4-phenoxyquinazoline 193001-79-5P, 4-(4-Chloro-2-fluorophenoxy)-7-hydroxy-6-methoxyquinazoline 193001-80-8P, 7-Benzyloxy-4-(4-chloro-2-fluorophenoxy)-6-methoxyquinazoline 193002-14-1P, 7-Benzyloxy-3,4-dihydroquinazolin-4-one 193002-18-5P, 2-[N-Methyl-N-(pyridazin-4-yl)amino]ethanol 193002-19-6P, 2-[N-(3,6-Dichloropyridazin-4-yl)-N-methylamino]ethanol 193002-24-3P, 7-Benzyloxy-6-methoxy-3-[(pivaloyloxy)methyl]-3,4-dihydroquinazolin-4-one 193002-25-4P, 7-Hydroxy-6-methoxy-3-[(pivaloyloxy)methyl]-3,4-dihydroquinazolin-4-one 193002-30-1P, 4-Chloro-7-[2-(imidazol-1-yl)ethoxy]-6-methoxyquinazoline 193002-31-2P, 7-[2-(Imidazol-1-yl)ethoxy]-6-methoxy-3-[(pivaloyloxy)methyl]-3,4-dihydroquinazolin-4-one 193002-32-3P, 7-[2-(Imidazol-1-yl)ethoxy]-6-methoxy-3,4-dihydroquinazolin-4-one 196194-61-3P, 6-Methoxy-7-(3-morpholinopropoxy)-4-phenoxyquinazoline 196194-62-4P, 6-Methoxy-7-(3-morpholinopropoxy)-3,4-dihydroquinazolin-4-one 196194-78-2P, 4-Chloro-6-methoxy-7-(2-piperidinoethoxy)quinazoline hydrochloride 196194-79-3P, 6-Methoxy-4-phenoxy-7-(2-piperidinoethoxy)quinazoline 196194-80-6P, 6-Methoxy-7-(2-piperidinoethoxy)-3,4-dihydroquinazolin-4-one 196195-13-8P, 4-Chloro-6-methoxy-7-(3-morpholinopropoxy)quinazoline

199327-69-0P, 4-Chloro-6-methoxy-7-[3-(pyrrolidin-1-yl)propoxy]quinazoline 199327-71-4P, 3-Methoxy-4-[3-(pyrrolidin-1-yl)propoxy]benzoic acid hydrochloride 199327-72-5P, 5-Methoxy-2-nitro-4-[3-(pyrrolidin-1-yl)propoxy]benzoic acid hydrochloride 199327-73-6P, 5-Methoxy-2-nitro-4-[3-(pyrrolidin-1-yl)propoxy]benzamide 199327-74-7P, 2-Amino-5-methoxy-4-[3-(pyrrolidin-1-yl)propoxy]benzamide hydrochloride 199327-75-8P, 4-Hydroxy-6-methoxy-7-[3-(pyrrolidin-1-yl)propoxy]quinazoline 199328-74-0P, 4-Chloro-6-methoxy-7-[2-(2-methoxyethoxy)ethoxy]quinazoline 199328-77-3P, 6-Methoxy-7-[2-(2-methoxyethoxy)ethoxy]-3-[(pivaloyloxy)methyl]-3,4-dihydroquinazolin-4-one 205194-11-2P, (R)-(1-Methylpiperidin-3-yl)methanol 205194-12-3P, (R)-Ethyl 1-methylpiperidine-3-carboxylate 205194-13-4P, (E)-4-(Pyrrolidin-1-yl)but-2-en-1-ol 205194-33-8P, 3-(1,1-Dioxothiomorpholino)-1-propanol 263400-83-5P, 4-Chloro-6-methoxy-7-[(1-methylpiperidin-3-yl)methoxy]quinazoline 263400-84-6P, 4-(4-Chloro-2-fluorophenoxy)-6-methoxy-7-[(1-methylpiperidin-3-yl)methoxy]quinazoline 263400-85-7P, 6-Methoxy-7-[(1-methylpiperidin-3-yl)methoxy]-3,4-dihydroquinazolin-4-one 264208-51-7P, 7-[3-(4-Methylpiperazin-1-yl)propoxy]-6-methoxy-3-[(pivaloyloxy)methyl]-3,4-dihydroquinazolin-4-one 264208-53-9P, 6-Methoxy-7-[3-(4-methylpiperazin-1-yl)propoxy]-3,4-dihydroquinazolin-4-one 264208-55-1P, 4-Chloro-6-methoxy-7-[3-(4-methylpiperazin-1-yl)propoxy]quinazoline 264208-58-4P, Ethyl 3-methoxy-4-((1-tert-butyloxycarbonylpiperidin-4-yl)methoxy)benzoate 264208-60-8P, Ethyl 3-methoxy-4-((1-methylpiperidin-4-yl)methoxy)benzoate 264208-63-1P, Ethyl 3-methoxy-4-((1-methylpiperidin-4-yl)methoxy)-6-nitrobenzoate 264208-66-4P, Ethyl 6-amino-3-methoxy-4-((1-methylpiperidin-4-yl)methoxy)benzoate 264208-69-7P, 6-Methoxy-7-[(1-methylpiperidin-4-yl)methoxy]-3,4-dihydroquinazolin-4-one 264208-72-2P, 4-Chloro-6-methoxy-7-[(1-methylpiperidin-4-yl)methoxy]quinazoline 264208-86-8P, 6-Methoxy-3-[(pivaloyloxy)methyl]-7-[(1-tert-butyloxycarbonylpiperidin-4-yl)methoxy]-3,4-dihydroquinazolin-4-one 264208-92-6P, 6-Methoxy-7-[[1-(2-methylsulfonylethyl)piperidin-4-yl]methoxy]-3-[(pivaloyloxy)methyl]-3,4-dihydroquinazolin-4-one 264208-95-9P, 6-Methoxy-7-[[1-(2-methylsulfonylethyl)piperidin-4-yl]methoxy]-3,4-dihydroquinazolin-4-one 264208-98-2P, 4-Chloro-6-methoxy-7-((1-(2-methylsulfonylethyl)piperidin-4-yl)methoxy)quinazoline 264209-07-6P, 6-Methoxy-7-(3-methylsulfonylpropoxy)-3-[(pivaloyloxy)methyl]-3,4-dihydroquinazolin-4-one 264209-09-8P, 6-Methoxy-7-(3-methylsulfonylpropoxy)-3,4-dihydroquinazolin-4-one 264209-11-2P, 4-Chloro-6-methoxy-7-(3-methylsulfonylpropoxy)quinazoline 288383-30-2P, 4-Chloro-7-[3-(1,1-dioxothiomorpholino)propoxy]-6-methoxyquinazoline 288383-31-3P, 4-(4-Chloro-2-fluorophenoxy)-7-[3-(1,1-dioxothiomorpholino)propoxy]-6-methoxyquinazoline 288383-32-4P, 7-[3-(1,1-Dioxothiomorpholino)propoxy]-6-methoxy-3,4-dihydroquinazolin-4-one 288383-36-8P, 6-Methoxy-7-[(piperidin-4-yl)methoxy]-3-[(pivaloyloxy)methyl]-3,4-dihydroquinazolin-4-one hydrochloride 288383-62-0P, 5-Hydroxy-2-trifluoromethylindole 288383-69-7P, 2-[N-(2-Methoxyethyl)-N-methylamino]ethanol 288383-71-1P, 4-Chloro-6-methoxy-7-(3-piperidinopropoxy)quinazoline 288383-72-2P, 7-(3-Bromopropoxy)-6-methoxy-3-[(pivaloyloxy)methyl]-3,4-dihydroquinazolin-4-one 288383-73-3P, 6-Methoxy-7-(3-piperidinopropoxy)-3-[(pivaloyloxy)methyl]-3,4-dihydroquinazolin-4-one 288383-74-4P, 6-Methoxy-7-(3-piperidinopropoxy)-3,4-dihydroquinazolin-4-one 288383-77-7P, 7-(2-Carboxyvinyl)-6-methoxy-4-(2-methylindol-5-yloxy)quinazoline 288383-78-8P, 4-(4-Chloro-2-fluorophenoxy)-6-methoxy-7-(trifluoromethylsulfonyloxy)quinazoline 288383-79-9P, 4-(4-Chloro-2-fluorophenoxy)-6-methoxy-7-[2-(tert-butoxycarbonyl)vinyl]quinazoline 288383-80-2P, 7-(2-Carboxyvinyl)-4-(4-chloro-2-fluorophenoxy)-6-methoxyquinazoline 288383-85-7P,

7-Hydroxy-4-(2-methylindol-5-yloxy)quinazoline 288383-86-8P, 7-Benzyloxy-4-chloroquinazoline 288383-87-9P, 7-Benzyloxy-4-(2-methylindol-5-yloxy)quinazoline 288383-91-5P, 4-(2,3-Dimethylindol-5-yloxy)-7-hydroxy-6-methoxyquinazoline 288383-93-7P, 7-Benzyloxy-4-(2,3-dimethylindol-5-yloxy)-6-methoxyquinazoline 288384-13-4P, 3-(Ethylsulfonyl)-1-propanol 288384-18-9P, 4-(2,3-Dimethylindol-5-ylamino)-7-hydroxy-6-methoxyquinazoline 288384-20-3P, 7-Benzyloxy-4-(2,3-dimethylindol-5-ylamino)-6-methoxyquinazoline 288384-22-5P, 3-(tert-Butyldimethylsilyloxy)-1-(1H-1,2,4-triazolyl)propane 288384-23-6P 288384-41-8P, 4-Chloro-6-methoxy-7-[3-(N-methyl-N-methylsulfonylamino)propoxy]quinazoline 288384-44-1P, 4-(4-Bromo-2-fluorophenoxy)-7-[3-(N-tert-butoxycarbonylamino)propoxy]-6-methoxyquinazoline 288384-45-2P, 7-(3-Aminopropoxy)-4-(4-bromo-2-fluorophenoxy)-6-methoxyquinazoline 288384-46-3P, 4-(4-Bromo-2-fluorophenoxy)-6-methoxy-7-[3-(N-methylsulfonylamino)propoxy]quinazoline 288384-47-4P, 4-(4-Bromo-2-fluorophenoxy)-6-methoxy-7-[3-(N-methyl-N-methylsulfonylamino)propoxy]quinazoline 288384-48-5P 288384-53-2P, 2-Chloro-3-fluoro-7-methoxyquinoline 288384-54-3P, 3-Fluoro-7-methoxyquinoline 288384-55-4P, 3-Fluoro-7-hydroxyquinoline 288384-56-5P, 3-Fluoro-7-hydroxy-2-methylquinoline 288384-58-7P, 3-Fluoro-7-methoxy-2-methylquinoline 288384-60-1P, 7-(2,3-Epoxypropoxy)-6-methoxy-4-(2-methylindol-5-yloxy)quinazoline 288384-61-2P, 5-Hydroxy-6-trifluoromethylindole 288384-62-3P, 5-Benzyloxy-2-nitro-4-(trifluoromethyl)benzeneacetonitrile 288384-66-7P, Ethyl 7-chloro-5-hydroxyindole-2-carboxylate 288384-68-9P, Ethyl 7-chloro-5-methoxyindole-2-carboxylate 288384-72-5P 288384-74-7P, 4-(4-Chloro-2-fluorophenoxy)-6-methoxy-7-[3-(4-methylpiperazin-1-yl)propoxy]quinazoline 288384-77-0P, 4-Chloro-6-methoxy-7-(2-piperidinoethoxy)quinazoline 288384-91-8P, 2-Chloro-5-hydroxybenzimidazole 288384-98-5P, 3-Cyano-7-hydroxyquinoline 288385-08-0P, 6-Methoxy-7-(3-morpholinopropoxy)-4-[(1-tert-butoxycarbonyl-1,2,3,4-tetrahydroquinolin-6-yl)oxy]quinazoline 288385-13-7P, 6-Hydroxy-4-(1-tert-butoxycarbonyl)-1,2,3,4-tetrahydroquinoline 288385-15-9P, 4-((1-tert-Butoxycarbonyl-2,3-dihydroindol-5-yl)oxy)-6-methoxy-7-[3-(pyrrolidin-1-yl)propoxy]quinazoline 288385-24-0P, 4-((1-tert-Butoxycarbonyl-2,3-dihydroindol-5-yl)oxy)-6-methoxy-7-((1-methylpiperidin-4-yl)methoxy)quinazoline 288385-40-0P, 7-Hydroxy-4-(indol-5-ylamino)-6-methoxyquinazoline 288385-42-2P, 7-Benzyloxy-4-(indol-5-ylamino)-6-methoxyquinazoline hydrochloride 288385-46-6P, 7-Hydroxy-6-methoxy-4-(2-methylindol-5-ylamino)quinazoline 288385-48-8P, 7-Benzyloxy-6-methoxy-4-(2-methylindol-5-ylamino)quinazoline hydrochloride 288385-56-8P, 3-[(4-Methyl-4H-1,2,4-triazol-3-yl)sulfanyl]propan-1-ol 288385-69-3P, 3-[[N-(2,6-Dimethyl-4-pyridyl)-N-methyl]amino]propan-1-ol 288385-85-3P, 4-Chloro-6-methoxy-7-[(1-(cyanomethyl)piperidin-4-yl)methoxy]quinazoline 288385-87-5P, 6-Methoxy-7-(piperidin-4-ylmethoxy)-3-[(pivaloyloxy)methyl]-3,4-dihydroquinazolin-4-one 288385-88-6P, 4-Fluoro-5-hydroxy-2-methylindole 288385-89-7P, 4-Fluoro-5-methoxyindole 288385-90-0P, 4-Fluoro-5-methoxy-1-tert-butoxycarbonylindole 288385-91-1P, 6-Fluoro-5-methoxy-1-tert-butoxycarbonylindole 288385-92-2P, 6-Fluoro-5-methoxy-2-methylindole 288385-93-3P, 4-Fluoro-5-methoxy-2-methylindole 288385-96-6P, 1,2-Difluoro-3-(2,2-dimethoxypropyl)-4-nitrobenzene 288385-98-8P, 3-Acetylmethyl-1-benzyloxy-2-fluoro-4-nitrobenzene 288385-99-9P, 3-Acetylmethyl-2-fluoro-1-methoxy-4-nitrobenzene 288386-02-7P, 4-Chloro-6-methoxy-7-[2-(1-methylpiperidin-4-yl)ethoxy]quinazoline 288386-04-9P, 4-Fluoro-5-hydroxyindole 288386-07-2P, 7-[2-(1-(tert-Butoxycarbonyl)piperidin-4-yl)ethoxy]-6-methoxy-3-[(pivaloyloxy)methyl]-3,4-dihydroquinazolin-4-one 288386-09-4P, 7-[2-(Piperidin-4-yl)ethoxy]-6-methoxy-3-

[(pivaloyloxy)methyl]-3,4-dihydroquinazolin-4-one 288386-11-8P, 7-[2-(1-Methylpiperidin-4-yl)ethoxy]-6-methoxy-3-[(pivaloyloxy)methyl]-3,4-dihydroquinazolin-4-one 288386-13-0P, 7-[2-(1-Methylpiperidin-4-yl)ethoxy]-6-methoxy-3,4-dihydroquinazolin-4-one 288386-15-2P, 6-Fluoro-5-hydroxyindole 288386-20-9P 288386-22-1P, 5-Cyanomethyl-2-fluoro-4-nitrobenzyloxybenzene 288386-29-8P, 6-Fluoro-5-hydroxy-2-methylindole 288386-37-8P, (R)-7-[2-Acetoxy-3-(pyrrolidin-1-yl)propoxy]-4-(4-fluoro-2-methylindol-5-yloxy)-6-methoxyquinazoline 288386-39-0P, (R)-7-(Oxiran-2-ylmethoxy)-6-methoxy-3-[(pivaloyloxy)methyl]-3,4-dihydroquinazolin-4-one 288386-41-4P, (R)-7-(2-Hydroxy-3-(pyrrolidin-1-yl)propoxy)-6-methoxy-3-((pivaloyloxy)methyl)-3,4-dihydroquinazolin-4-one 288386-43-6P, (R)-7-[2-Hydroxy-3-(pyrrolidin-1-yl)propoxy]-6-methoxy-3,4-dihydroquinazolin-4-one 288386-44-7P, (R)-7-[2-Acetoxy-3-(pyrrolidin-1-yl)propoxy]-6-methoxy-3,4-dihydroquinazolin-4-one 288386-46-9P, (R)-7-[2-Acetoxy-3-(pyrrolidin-1-yl)propoxy]-4-chloro-6-methoxyquinazoline 288386-66-3P 288386-71-0P, (R)-6-Methoxy-4-(2-methylindol-5-yloxy)-7-(oxiran-2-ylmethoxy)quinazoline 288386-75-4P, 7-Benzyloxy-6-methoxy-4-(3-methylindol-5-yloxy)quinazoline 288387-15-5P, 4-Bromo-5-hydroxyindole 288387-21-3P, (R)-4-(Indol-5-yloxy)-6-methoxy-7-(oxiran-2-ylmethoxy)quinazoline 288387-27-9P, (S)-4-(Indol-5-yloxy)-6-methoxy-7-(oxiran-2-ylmethoxy)quinazoline 288387-39-3P, (S)-6-Methoxy-4-(2-methylindol-5-yloxy)-7-(oxiran-2-ylmethoxy)quinazoline 288387-48-4P, Ethyl 5-hydroxy-4-nitroindole-2-carboxylate 288387-49-5P, 5-Methoxy-4-nitroindole-2-carboxylic acid 288387-52-0P, 7-(3-Bromopropoxy)-4-(1H-indol-5-yloxy)-6-methoxyquinazoline 288387-54-2P, (S)-5-(p-Toluenesulfonylmethyl)-1-methyl-2-pyrrolidinone 288387-58-6P, (R)-5-(p-Toluenesulfonylmethyl)-2-pyrrolidinone
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of quinazolines as angiogenesis inhibitors by cyclization of 2-aminobenzamides and subsequent derivatization)

IT 59-31-4, 2-Hydroxyquinoline 86-79-3, 2-Hydroxycarbazole 87-13-8, Diethyl ethoxymethylenemalonate 90-15-3, 1-Naphthol 98-00-0, 2-Furanmethanol 100-37-8, N,N-Diethylethanolamine 100-55-0, 3-Hydroxymethyl pyridine 102-51-2, 4-Methoxy-1,2-phenylenediamine 104-58-5, 1-(3-Hydroxypropyl)piperidine 107-13-1, 2-Propenenitrile, reactions 108-01-0, N,N-Dimethylethanolamine 109-01-3, 1-Methylpiperazine 109-64-8, 1,3-Dibromopropane 109-70-6, 1-Bromo-3-chloropropane 109-83-1, 2-(Methylamino)ethanol 110-65-6, 2-Butyne-1,4-diol 110-89-4, Piperidine, reactions 110-91-8, Morpholine, reactions 111-77-3, 2-(2-Methoxyethoxy)ethanol 112-35-6, Triethylene glycol monomethyl ether 121-34-6, 4-Hydroxy-3-methoxybenzoic acid 123-00-2, 4-(3-Aminopropyl)morpholine 123-56-8, Pyrrolidine-2,5-dione 135-19-3, 2-Hydroxynaphthalene, reactions 137-00-8, 5-(2-Hydroxyethyl)-4-methylthiazole 140-53-4, 4-Chlorophenylacetonitrile 140-88-5 141-97-9, Ethyl acetoacetate 156-87-6, 3-Amino-1-propanol 177-11-7, 4,4-(Ethylenedioxy)piperidine 288-36-8, 1,2,3-Triazole 288-88-0, 1H-1,2,4-Triazole 348-62-9, 4-Chloro-2-fluorophenol 403-19-0, 2-Fluoro-4-nitrophenol 455-93-6, 2-Fluoro-4-nitroanisole 505-10-2, 3-(Methylthio)-1-propanol 533-30-2, 6-Aminobenzothiazole 536-90-3 578-67-6, 5-Hydroxyquinoline 580-16-5, 6-Hydroxyquinoline 580-20-1, 7-Hydroxyquinoline 582-17-2, 2,7-Dihydroxynaphthalene 617-05-0, Ethyl 3-methoxy-4-hydroxybenzoate 622-40-2, 4-(2-Hydroxyethyl)morpholine 622-93-5, 3-(N,N-Diethylamino)-1-propanol 627-18-9, 3-Bromo-1-propanol 627-30-5, 3-Chloropropan-1-ol 628-89-7, 2-(2-Chloroethoxy)ethanol 771-69-7, 1,2,3-Trifluoro-4-nitrobenzene 777-37-7, 2-Chloro-5-nitrotrifluoromethylbenzene 828-94-4, 2,3-Dimethyl-5-methoxyindole 1076-74-0, 5-Methoxy-2-

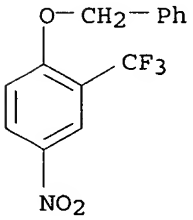
methylindole 1122-58-3, 4-Dimethylaminopyridine 1125-40-2, 3-Methyl-5-hydroxyindole 1126-09-6, Ethyl 4-piperidinecarboxylate 1458-63-5, 1-(3-Chloropropyl)piperidine 1484-84-0, 2-(2-Hydroxyethyl)piperidine 1615-14-1, 2-(Imidazol-1-yl)ethanol 1663-39-4 **1953-54-4**, 5-Hydroxyindole 2008-75-5, 1-(2-Chloroethyl)piperidine hydrochloride 2380-86-1, 6-Hydroxyindole 2380-94-1, 4-Hydroxyindole 2439-68-1, 5-Benzyloxy-1-methylindole 2941-62-0, 6-Amino-2-methylbenzothiazole 2955-88-6, 1-(2-Hydroxyethyl)pyrrolidine 3040-44-6, 1-(2-Hydroxyethyl)piperidine 3132-64-7, Epibromohydrin 3179-63-3, 3-(N,N-Dimethylamino)propanol 3273-14-1, 2-(1H-1,2,4-Triazol-1-yl)ethanol 3445-11-2, 1-(2-Hydroxyethyl)-2-pyrrolidinone 3512-75-2, 4-Chloro-2,6-dimethylpyridine 3598-13-8, 4-Chlorophenoxyacetonitrile 3647-69-6, 4-(2-Chloroethyl)morpholine hydrochloride 3680-02-2, Methyl vinyl sulfone 4076-31-7, 2-[2-(4-Methylpiperazin-1-yl)ethoxy]ethanol 4572-03-6, 1-(3-Aminopropyl)-4-methylpiperazine 4769-96-4, 6-Nitroindole 4790-04-9, 5-Benzyloxy-6-methoxyindole 4792-58-9, Ethyl 5-methoxyindole-2-carboxylate 4897-50-1, 4-Piperidinopiperidine 5050-41-9, 1-(2-Chloroethyl)pyrrolidine 5192-03-0, 5-Aminoindole 5344-27-4, 4-(2-Hydroxyethyl)pyridine 5653-40-7, 4,5-Dimethoxyanthranilic acid 6293-56-7, 3-(2-Hydroxyethyl)pyridine 6320-42-9, 7-Hydroxy-2-methylchromone 6482-24-2, 2-Bromoethyl methyl ether 6967-12-0, 6-Aminoindazole 7154-73-6, 1-(2-Aminoethyl)pyrrolidine 7384-07-8, 3-Hydroxycarbazole 7570-47-0, 2-Methyl-5-nitroindole 7570-49-2, 5-Amino-2-methylindole 7583-53-1, (1-Methylpiperidin-3-yl)methanol 10344-42-0, 4-Bromo-3,6-dichloropyridazine 14268-66-7, 3,4-(Methylenedioxy)aniline 15463-09-9, 7-Hydroxy-4-methylquinoline 15965-54-5, 2-Chloro-5-methoxybenzimidazole 16499-57-3, 7-Fluoro-3,4-dihydroquinazolin-4-one 16712-58-6, 5-Amino-2,3-dimethylindole 17342-08-4 18190-44-8, 1-(2-Hydroxyethyl)pyrrolidin-2,5-dione 18721-61-4, 3-(Ethylthio)propanol 18994-70-2, 2-(1-Methylimidazol-2-yl)ethanol 19335-11-6, 5-Aminoindazole 19748-66-4, 3-Pyrrolidinopropan-1-ol 20845-32-3, 4-Hydroxymethyl-1-methyl-2-piperidone 21598-06-1, 5-Hydroxy-2-indolecarboxylic acid 22159-27-9, 1-(3-Hydroxypropyl)-2-methylimidazole 23159-07-1, 1-(3-Aminopropyl)pyrrolidine 24332-20-5, 1,1,2-Trimethoxyethane 24425-40-9, 5-Aminoindan 24854-43-1, 4-Methyl-4H-1,2,4-triazole-3-thiol 25137-01-3, (R)-Ethyl nipecotate 25888-06-6, 1,2-Dimethyl-5-hydroxyindole 26438-50-6, 3,4-Dihydro-4-methyl-2H-1,4-benzoxazin-6-ol 29242-84-0, 2-Chloro-4-methoxyaniline 34381-71-0, (S)-2-(Hydroxymethyl)-1-methylpyrrolidine 39743-20-9, 3-(Pyrrolidin-1-yl)propyl chloride 42055-15-2, 3-(N-Methylamino)propan-1-ol 51086-19-2 53412-38-7, 6-Hydroxy-3,4-dihydro-2H-1,4-benzoxazin-3-one 54584-22-4, 6-Hydroxy-2-methylindole 57561-39-4 58885-58-8, 3-(N-tert-Butoxycarbonylamino)propanol 60547-98-0, 2-Amino-4-benzyloxy-5-methoxybenzamide 62012-15-1, 1-(3-Hydroxypropyl)pyrrolidin-2-one 66673-40-3, (R)-5-Hydroxymethyl-2-pyrrolidinone 68867-14-1, 5-Hydroxy-2-methylbenzothiazole 72107-05-2, 2,2,4-Trimethyl-1,2-dihydroquinolin-6-ol 72365-58-3, 2,4-Dimethyl-7-hydroxyquinoline 86450-38-6, 4-(2-Hydroxyethoxy)pyridine 98549-88-3, 5-Hydroxy-1H-pyrrolo[2,3-b]pyridine 104863-67-4, N-Methyl-N-methoxytrifluoroacetamide 109736-44-9, 2-[N-Methyl-N-(4-pyridyl)amino]ethanol 116141-68-5, 5,5-Dimethyl-1,3-dioxane-2-ethanol 129822-42-0, (4-Methoxy-2-methylphenyl)carbamic acid 1,1-dimethylethyl ester 151782-79-5, 7-Hydroxy-4-trifluoromethylquinoline 165112-03-8, 7-Hydroxy-2-methylquinoline 175609-41-3, 3-Fluoro-7-methoxyquinolin-2(1H)-one 178984-56-0, 7-Benzyloxy-4-chloroquinoline 183208-36-8, 5-Methoxy-1H-pyrrolo[2,3-b]pyridine 288383-51-7, 4-Chloro-6-methoxy-7-(1-methylpiperidin-4-yloxy)quinazoline 288383-83-5, 6-Methoxy-4-((2-

methylindol-5-yl)oxy)-7-[2-(N-methyl-N-tert-butoxycarbonylamino)ethoxy]quinazoline 288384-43-0, 4-(4-Bromo-2-fluorophenoxy)-7-hydroxy-6-methoxyquinazoline 288384-73-6, 4-(4-Chloro-2-fluorophenoxy)-7-hydroxy-6-methoxyquinazoline trifluoroacetate 288385-51-3, 3-(1H-1,2,3-Triazol-1-yl)propan-1-ol 288386-62-9, 4-Chloro-6-methoxy-7-[3-(1H-1,2,4-triazol-1-yl)propoxy]quinazoline 288386-86-7, 3-(1,1-Dioxothiomorpholino)propoxy tosylate 288387-56-4, (S)-5-(p-Toluenesulfonylmethyl)-2-pyrrolidinone 288387-63-3, 7-Hydroxy-4-thiomethylquinazoline
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of quinazolines as angiogenesis inhibitors by cyclization of 2-aminobenzamides and subsequent derivatization)

IT **39062-69-6P**, 2-Benzyloxy-5-nitrotrifluoromethylbenzene
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of quinazolines as angiogenesis inhibitors by cyclization of 2-aminobenzamides and subsequent derivatization)

RN 39062-69-6 HCAPLUS

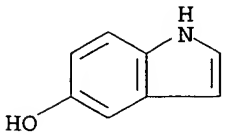
CN Benzene, 4-nitro-1-(phenylmethoxy)-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)



IT **1953-54-4**, 5-Hydroxyindole
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of quinazolines as angiogenesis inhibitors by cyclization of 2-aminobenzamides and subsequent derivatization)

RN 1953-54-4 HCAPLUS

CN 1H-Indol-5-ol (9CI) (CA INDEX NAME)



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DOCUMENT NUMBER: 131:31808

TITLE: Preparation of phthalic acid diamides as agricultural and horticultural insecticides

INVENTOR(S): Tohnishi, Masanori; Nakao, Hayami; Kohno, Eiji; Nishida, Tateki; Furuya, Takashi; Shimizu, Toshiaki; Seo, Akira; Sakata, Kazuyuki; Fujioka, Shinsuke; Kanno, Hideo

PATENT ASSIGNEE(S): Nihon Nohyaku Co., Ltd., Japan

SOURCE: Eur. Pat. Appl., 237 pp.
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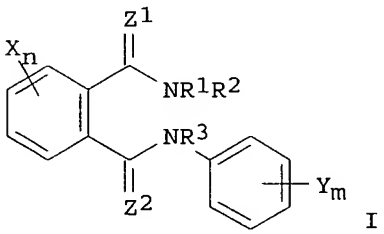
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 919542	A2	19990602	EP 1998-122107	19981123
EP 919542	A3	20000412		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
TW 515786	B	20030101	TW 1998-87118850	19981113
AU 9893292	A1	19990624	AU 1998-93292	19981120
AU 712421	B2	19991104		
ZA 9810677	A	19990526	ZA 1998-10677	19981123
CZ 291181	B6	20030115	CZ 1998-3799	19981123
EP 1447396	A1	20040818	EP 2004-9422	19981123
R: CH, DE, DK, ES, FR, GB, IT, LI, FI				
EG 22230	A	20021130	EG 1998-1466	19981124
CN 1222506	A	19990714	CN 1998-122688	19981125
CN 1068584	B	20010718		
JP 11240857	A2	19990907	JP 1998-350768	19981125
BR 9805060	A	20000321	BR 1998-5060	19981125
PRIORITY APPLN. INFO.:			JP 1997-339393 A	19971125
			EP 1998-122107 A3	19981123

OTHER SOURCE(S): MARPAT 131:31808
GI



I

AB The title compds. [I; R1-R3 = H, CN, cycloalkyl, etc.; X = H, CN, NO2, etc.; n = 1-4; Y = H, halo, CN, etc.; m = 1-5; Z1, Z2 = O, S] which show excellent activities for controlling injurious insects, were prepared Thus, reaction of 3-nitro-2-ethoxycarbonylbenzoyl chloride with 4-chloro-2-methylaniline in the presence of Et3N in THF followed by treatment of the resulting Et 6-nitro-N-(4-chloro-2-methylphenyl)phthalamate with isopropylamine in dioxane afforded I [R1 = iPr; R2 = R3 = H; X = 3-NO2; Y = 2-Me-4-Cl; Z1 = Z2 = O] which showed excellent insecticidal effect (100% mortality) against diamondback moth and common cutworm.

IC ICM C07C233-64
ICS C07C235-42; C07C317-32; C07C323-42; C07D295-192; A01N037-18; A01N043-00; A01N043-84; A01N057-00
CC 25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 5
IT 16497-37-3P 16497-38-4P 226958-87-8P 226958-88-9P 226958-89-0P 226958-90-3P 226958-91-4P 226958-92-5P 226958-93-6P 226958-94-7P

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RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of phthalic acid diamides as agricultural and horticultural insecticides)

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(preparation of phthalic acid diamides as agricultural and horticultural insecticides)

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RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of phthalic acid diamides as agricultural and horticultural insecticides)

IT **95-69-2**, 4-Chloro-2-methylaniline 117-21-5, 3-Chlorophthalic anhydride 461-82-5, 4-Trifluoromethoxyaniline 641-70-3 2253-73-8, Isopropyl isothiocyanate 28394-52-7 28418-88-4, 3-Iodophthalic anhydride 39211-40-0 39211-57-9 226979-96-0 226979-97-1 226979-98-2

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of phthalic acid diamides as agricultural and horticultural insecticides)

IT **226960-70-9P 226961-60-0P 226963-22-0P 226963-84-4P 226966-20-7P**

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of phthalic acid diamides as agricultural and horticultural insecticides)

RN 226960-70-9 HCAPLUS

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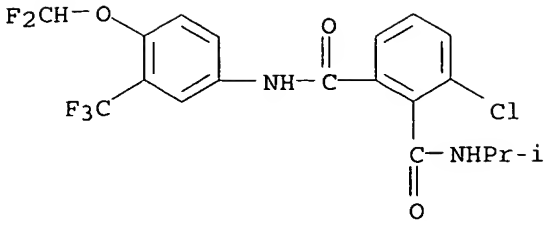

RN 226961-60-0 HCAPLUS
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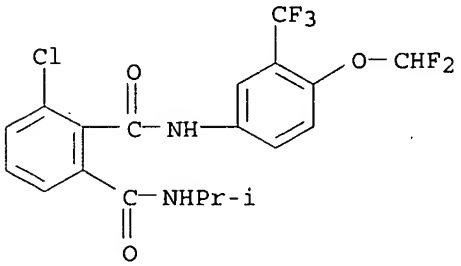

RN 226963-22-0 HCAPLUS
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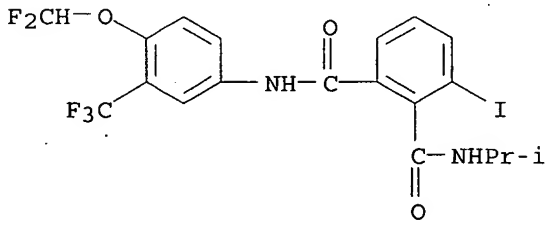

RN 226963-84-4 HCAPLUS
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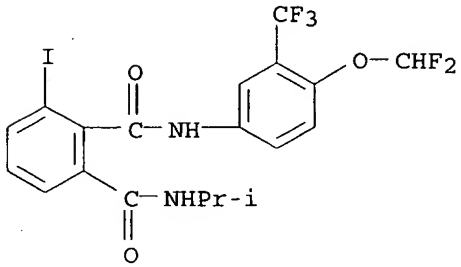
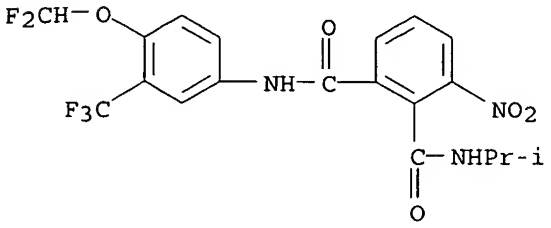
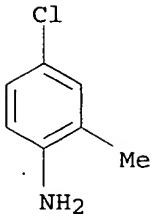


RN 226966-20-7 HCAPLUS
CN 1,2-Benzenedicarboxamide, N1-[4-(difluoromethoxy)-3-(trifluoromethyl)phenyl]-N2-(1-methylethyl)-3-nitro- (9CI) (CA INDEX NAME)



IT **95-69-2**, 4-Chloro-2-methylaniline
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of phthalic acid diamides as agricultural and horticultural insecticides)
RN 95-69-2 HCAPLUS
CN Benzenamine, 4-chloro-2-methyl- (9CI) (CA INDEX NAME)



L33 ANSWER 15 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:192042 HCAPLUS
DOCUMENT NUMBER: 126:185882
TITLE: Substituted cinnamic acid guanidides, process for their preparation, their use as cardiovascular medicament or diagnostic agent, as well as medicament containing them
INVENTOR(S): Schwark, Jan-Robert; Brendel, Joachim; Kleemann, Heinz-Werner; Lang, Hans-Jochen; Weichert, Andreas; Albus, Udo; Scholz, Wolfgang
PATENT ASSIGNEE(S): Hoechst A.-G., Germany
SOURCE: Eur. Pat. Appl., 19 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 755919	A2	19970129	EP 1996-111665	19960719
EP 755919	A3	19970409		
EP 755919	B1	19991117		

R: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE

DE 19527305	A1	19970130	DE 1995-19527305	19950726
PL 183439	B1	20020628	PL 1996-314279	19960516
AT 186720	E	19991215	AT 1996-111665	19960719
ES 2140765	T3	20000301	ES 1996-111665	19960719
CN 1145899	A	19970326	CN 1996-110200	19960723
CN 1062554	B	20010228		
AU 9660668	A1	19970130	AU 1996-60668	19960724
AU 704461	B2	19990422		
US 5883133	A	19990316	US 1996-686999	19960724
IL 118925	A1	20010808	IL 1996-118925	19960724
SK 282018	B6	20011008	SK 1996-965	19960724
CZ 289327	B6	20020116	CZ 1996-2184	19960724
CA 2182062	AA	19970127	CA 1996-2182062	19960725
NO 9603108	A	19970127	NO 1996-3108	19960725
ZA 9606313	A	19970211	ZA 1996-6313	19960725
JP 09052823	A2	19970225	JP 1996-196283	19960725
HR 960356	B1	20010228	HR 1996-960356	19960725
BR 9603179	A	20020409	BR 1996-3179	19960725
RU 2190601	C2	20021010	RU 1996-115333	19960725
TW 536531	B	20030611	TW 1996-85110279	19960823
GR 3032363	T3	20000427	GR 2000-400061	20000114

PRIORITY APPLN. INFO.: DE 1995-19527305 A 19950726

OTHER SOURCE(S): MARPAT 126:185882

AB Substituted cinnamic acid guanidides, such as E-3-(4-Me2NC6H4)CH:CMeCON:N(NH2)2, were prepared by the reaction of lithiated tri-Et 2-phosphonopropionate in hexane with 4-Me2NC6H4CHO, the resulting ester saponified, followed by reaction with cinnamic acid guanidide. These substituted cinnamic acid guanidides were tested as inhibitors for Na+/H+ exchange by rabbit erythrocytes, indicating their use as cardiovascular drugs or diagnostic agents.

IC ICM C07C279-22
ICS C07D213-65; C07D213-70; A61K031-155; A61K031-44

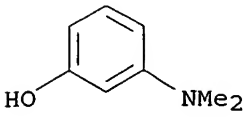
CC 25-9 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1

IT **99-07-0**, 3-Dimethylaminophenol 100-10-7, 4-(Dimethylamino)benzaldehyde 109-00-2, 3-Hydroxypyridine 459-57-4, 4-Fluorobenzaldehyde 539-15-1, 4-(2-Dimethylaminoethyl)phenol 3699-66-9, Triethyl 2-phosphonopropionate 4556-23-4, 4-Mercaptopyridine 26934-35-0, 4-(3-Dimethylaminopropoxy)benzaldehyde 58551-83-0, 2,4,6-Trifluorobenzaldehyde 67515-60-0, 4-Fluoro-3-trifluoromethylbenzaldehyde 132123-54-7, 3,4,5-Trifluorobenzaldehyde 148901-53-5, 3-Cyano-4-dimethylamino-2-fluorobenzaldehyde 187541-47-5 187541-52-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of substituted cinnamic acid guanidides)

IT 134294-41-0P 187541-48-6P 187541-49-7P 187541-50-0P 187541-51-1P 187541-54-4P **187541-55-5P** 187541-56-6P 187541-57-7P 187541-58-8P 187541-59-9P 187541-60-2P 187541-61-3P 187541-62-4P 187541-63-5P 187541-64-6P 187541-65-7P 187541-66-8P 187541-67-9P 187541-68-0P 187541-69-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for preparation of substituted cinnamic acid guanidides)

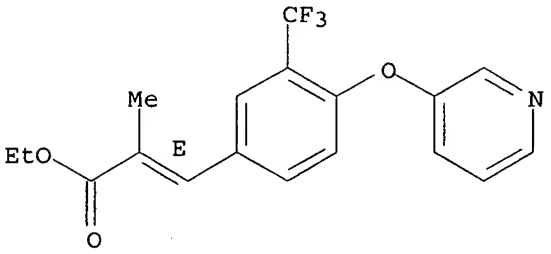
IT 187541-36-2P 187541-37-3P **187541-38-4P** 187541-39-5P 187541-40-8P 187541-41-9P 187541-42-0P 187541-43-1P 187541-44-2P 187541-45-3P 187541-46-4P 187541-70-4P
RL: IMF (Industrial manufacture); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and use as cardiovascular drugs or diagnostic agents)

IT **99-07-0**, 3-Dimethylaminophenol
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of substituted cinnamic acid guanidides)
RN 99-07-0 HCAPLUS
CN Phenol, 3-(dimethylamino)- (9CI) (CA INDEX NAME)



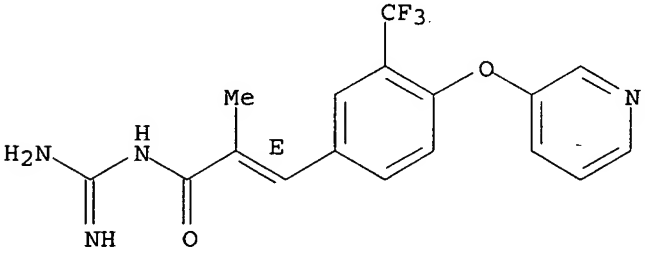
IT **187541-55-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for preparation of substituted cinnamic acid guanidides)
RN 187541-55-5 HCAPLUS
CN 2-Propenoic acid, 2-methyl-3-[4-(3-pyridinyloxy)-3-(trifluoromethyl)phenyl]-, ethyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



IT **187541-38-4P**
RL: IMF (Industrial manufacture); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and use as cardiovascular drugs or diagnostic agents)
RN 187541-38-4 HCAPLUS
CN 2-Propenamide, N-(aminoiminomethyl)-2-methyl-3-[4-(3-pyridinyloxy)-3-(trifluoromethyl)phenyl]-, dihydrochloride, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

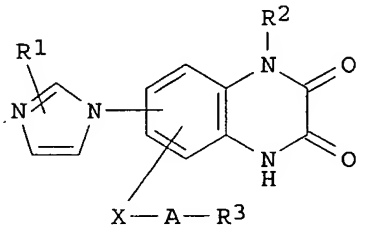


●2 HCl

L33 ANSWER 16 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:582559 HCAPLUS
DOCUMENT NUMBER: 122:314573
TITLE: Preparation of imidazolylquinoxalinedione derivatives as glutamate receptor antagonists
INVENTOR(S): Sakamoto, Shuichi; Shishikura, Jun-ichi; Iwata, Masahiro; Okada, Masamichi; Sasamata, Masao
PATENT ASSIGNEE(S): Yamparm, Japan
SOURCE: PCT Int. Appl., 103 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9426737	A1	19941124	WO 1994-JP758	19940511
W: AU, BB, BG, BR, BY, CA, CN, CZ, FI, GE, HU, JP, KG, KR, KZ, LK, LV, MD, MG, MN, MW, NO, NZ, PL, PT, RO, RU, SD, SI, SK, TJ, TT, UA, US, UZ, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9466903	A1	19941212	AU 1994-66903	19940511
PRIORITY APPLN. INFO.:			JP 1993-134033 A	19930512
			JP 1993-296525 A	19931126
			WO 1994-JP758 W	19940511

OTHER SOURCE(S): MARPAT 122:314573
GI



I

AB Title compds. I [R1 = H, alkyl; R2 = H, OH; X = O, NR4, S(O)m; R3 = alkyl, carboxy, or (un)substituted Ph, cycloalkyl or mono- or bicyclic heterocyclic group; R4 = H, alkyl; n = 0, 1, 2; A = direct bond, alkylene] and their pharmaceutically acceptable salts, useful as glutamate receptor antagonists, psychotropics, nerve cell protecting agents, and for treatment of brain ischemia, were prepared Thus, reduction of 5-(1H-imidazol-1-yl)-4-methoxy-2-nitroaniline with H in MeOH in the presence of PtO2 and HCl at room temp for 2.5 h followed by cyclocondensation with oxalic acid in aqueous HCl gave 6-(1H-imidazol-1-yl)-7-methoxyquinoxaline-2,3(1H,4H)-dione hydrochloride. 4-{[4-Hydroxy-7-(1H-imidazol-1-yl)-2,3-dioxo-1,2,3,4-tetrahydroquinoxalin-6-yl]oxymethyl}benzoic acid hydrochloride showed nerve cell protection activity in mice.
IC ICM C07D403-04
ICS A61K031-495
CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))

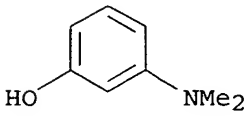
Section cross-reference(s): 1, 63

IT **99-07-0**, Phenol, 3-(dimethylamino)- 99-76-3, Benzoic acid, 4-hydroxy-, methyl ester 108-95-2, Phenol, reactions 109-00-2, 3-Pyridinol 119-36-8, Benzoic acid, 2-hydroxy-, methyl ester 144-62-7, Oxalic acid, reactions 288-32-4, 1H-Imidazole, reactions 617-05-0, Benzoic acid, 4-hydroxy-3-methoxy-, ethyl ester 619-08-9, Phenol, 2-chloro-4-nitro- 623-51-8, Acetic acid, mercapto-, ethyl ester 767-00-0, Benzonitrile, 4-hydroxy- 822-36-6, 1H-Imidazole, 4-methyl- 872-35-5, 1H-Imidazole-2-thiol 1679-07-8, Cyclopentanethiol 3943-74-6, Benzoic acid, 4-hydroxy-3-methoxy-, methyl ester 4892-02-8, Benzoic acid, 2-mercapto-, methyl ester 6302-65-4, Benzoic acid, 4-mercapto-, methyl ester 10041-02-8, Phenol, 4-(1H-imidazol-1-yl)- 16357-41-8, Benzoic acid, 3-chloro-4-hydroxy-, ethyl ester 19438-10-9, Benzoic acid, 3-hydroxy-, methyl ester 22479-95-4, 1,2-Benzenedicarboxylic acid, 4-hydroxy-, dimethyl ester 29490-19-5 29655-46-7, Carbamic acid, [2-(4-hydroxyphenyl)ethyl]-, phenylmethyl ester 51138-06-8, 5H-Tetrazole-5-thione, 1,2-dihydro-1-methyl-, sodium salt 51991-39-0 56069-35-3, Benzoic acid, 2-chloro-4-hydroxy-, ethyl ester 154164-63-3 163485-15-2 163485-18-5 163485-21-0 163485-24-3 163485-27-6 163485-30-1 163485-34-5 163485-43-6 163485-46-9 163485-53-8 163485-56-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of imidazolylquinoxalinedione derivs. as glutamate receptor antagonists)

IT 163484-52-4P 163484-53-5P 163484-54-6P 163484-55-7P 163484-56-8P 163484-57-9P 163484-58-0P 163484-59-1P 163484-60-4P 163484-61-5P 163484-62-6P 163484-63-7P 163484-64-8P 163484-65-9P 163484-66-0P 163484-67-1P 163484-68-2P 163484-69-3P 163484-70-6P 163484-71-7P 163484-72-8P 163484-73-9P 163484-75-1P 163484-76-2P 163484-77-3P 163484-78-4P 163484-79-5P 163484-80-8P 163484-81-9P 163484-82-0P 163484-83-1P 163484-84-2P 163484-85-3P 163484-86-4P 163484-87-5P 163484-89-7P 163484-90-0P 163484-91-1P 163484-92-2P 163484-93-3P 163484-94-4P 163484-95-5P 163484-96-6P 163484-97-7P
163484-98-8P 163484-99-9P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of imidazolylquinoxalinedione derivs. as glutamate receptor antagonists)

IT **99-07-0**, Phenol, 3-(dimethylamino)-
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of imidazolylquinoxalinedione derivs. as glutamate receptor antagonists)

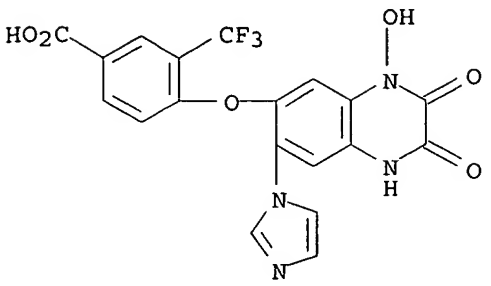
RN 99-07-0 HCAPLUS
CN Phenol, 3-(dimethylamino)- (9CI) (CA INDEX NAME)



IT **163484-98-8P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of imidazolylquinoxalinedione derivs. as glutamate receptor antagonists)

RN 163484-98-8 HCAPLUS
CN Benzoic acid, 4-[[1,2,3,4-tetrahydro-4-hydroxy-7-(1H-imidazol-1-yl)-2,3-

dioxo-6-quinoxalinyl]oxy]-3-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



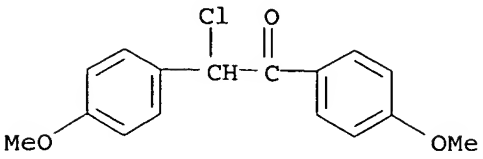
● HCl

L33 ANSWER 17 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1993:582847 HCAPLUS
DOCUMENT NUMBER: 119:182847
TITLE: Synthesis and nonlinear optical properties of donor-acceptor substituted triaryl azole derivatives
AUTHOR(S): Moylan, Christopher R.; Miller, Robert D.; Twieg, Robert J.; Betterton, Kathleen M.; Lee, Victor Y.; Matray, Tracy J.; Nguyen, Cattien
CORPORATE SOURCE: Almaden Res. Cent., IBM, San Jose, CA, 95120-6099, USA
SOURCE: Chemistry of Materials (1993), 5(10), 1499-508
CODEN: CMATEX; ISSN: 0897-4756
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A variety of optically nonlinear chromophores containing a 5-membered imidazole, oxazole, or thiozole ring were prepared and characterized. These consisted of 2,4,5-triphenyl-substituted azole heterocyclic systems in which the 2-aryl ring bore an electron-withdrawing substituent and the 4,5-aryl rings bore an electron-donating substituent. Addnl., some planar analogs, phenanthro[9,10-d]imidazoles, were also prepared and evaluated. The utility of these chromophores was dictated by their linear absorption wavelength and oscillator strength, microscopic optical nonlinearity, ground-state dipole moment, thermal stability, and solubility The trade offs between these structure-dependent properties were discussed with regard to exploitation of these chromophores as guest dyes in high-temperature thermoplastics.

CC 41-5 (Dyes, Organic Pigments, Fluorescent Brighteners, and Photographic Sensitizers)
IT **Dyes**
(preparation and nonlinear properties of, based on triarylazoles containing donor and acceptor substituents)
IT **71193-36-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with nitrothiobenzamide)
IT **71193-36-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with nitrothiobenzamide)
RN 71193-36-7 HCAPLUS

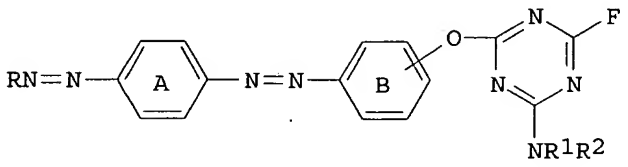
CN Ethanone, 2-chloro-1,2-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



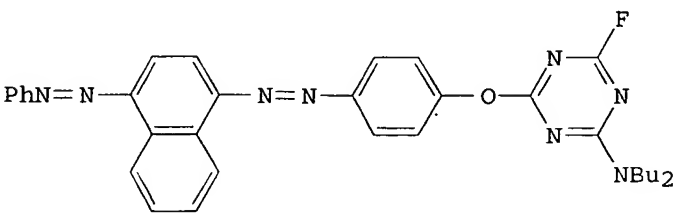
L33 ANSWER 18 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1983:424003 HCAPLUS
DOCUMENT NUMBER: 99:24003
TITLE: Reactive disazo dyes for cellulosic fibers
INVENTOR(S): Niwa, Toshio; Hihara, Toshio
PATENT ASSIGNEE(S): Mitsubishi Chemical Industries Co., Ltd. , Japan
SOURCE: Ger. Offen., 103 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3227134	A1	19830203	DE 1982-3227134	19820720
DE 3227134	C2	19900322		
JP 58013789	A2	19830126	JP 1981-113259	19810720
JP 01048945	B4	19891023		
JP 58109560	A2	19830629	JP 1981-208497	19811223
JP 03032586	B4	19910513		
JP 58134153	A2	19830810	JP 1982-15699	19820203
JP 03032587	B4	19910513		
GB 2105738	A1	19830330	GB 1982-20875	19820719
GB 2105738	B2	19850522		
US 4473499	A	19840925	US 1982-400201	19820720
CH 649093	A	19850430	CH 1982-4425	19820720
PRIORITY APPLN. INFO.:			JP 1981-113259	19810720
			JP 1981-208497	19811223
			JP 1982-15699	19820203

GI



I



II

AB Light- and wetfast yellow to red dyes for cellulosic textiles are described having the general formula I (R = benzene, 3-methyl-1-phenyl-5-pyrazolone, 2,6-diamino-3-cyano-4-methylpyridine, or acetoacetanilide moiety; R1, R2 = H or substituted or unsubstituted alkyl, or NR1R2 = heterocycle) with or without substituent(s) on the rings A and B. Thus, reaction of 4-[[4-(phenylazo)-1-naphthyl]azo]phenol [6253-10-7] with 2-(dibutylamino)-4,6-difluoro-s-triazine [84875-65-0] in N-methylpyrrolidone containing Et3N gave II [85401-48-5] which produced fast yellowish brown prints on 65:35 polyester-cotton fabric. Numerous other I (>200) are described.

IC C09B062-09; D06P003-66; D06P001-04

CC 41-3 (Dyes, Organic Pigments, Fluorescent Brighteners, and Photographic Sensitizers)

IT **Dyes, reactive**
(disazo compds., aminofluorotriazinyloxy group-containing, for cellulosic textiles)

IT
85399-37-7	85399-55-9	85399-56-0	85399-57-1	85399-58-2
85399-59-3	85399-60-6	85399-61-7	85399-62-8	85399-63-9
85399-64-0	85399-65-1	85399-66-2	85399-67-3	85399-68-4
85399-69-5	85399-70-8	85399-71-9	85399-72-0	85399-73-1
85399-74-2	85399-75-3	85399-76-4	85399-77-5	85399-78-6
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85399-84-4	85399-85-5	85399-86-6	85399-87-7	85399-88-8
85399-89-9	85399-90-2	85399-91-3	85399-92-4	85399-93-5
85399-94-6	85399-95-7	85399-96-8	85399-97-9	85399-98-0
85399-99-1	85400-00-6	85400-01-7	85400-02-8	85400-03-9
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85400-14-2	85400-15-3	85400-16-4	85400-17-5	85400-18-6
85400-23-3	85400-24-4	85400-25-5	85400-26-6	85400-27-7
85400-28-8	85400-29-9	85400-30-2	85400-31-3	85400-32-4
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85400-43-7	85400-44-8	85400-45-9	85400-46-0	85400-47-1
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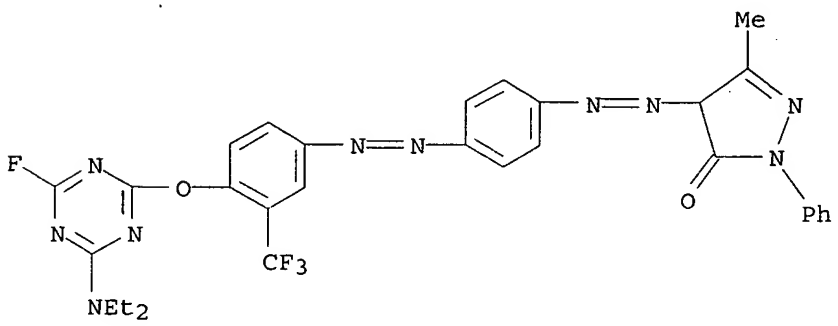
85400-92-6	85400-93-7	85400-94-8	85400-95-9	85401-00-9
85401-01-0	85401-02-1	85401-03-2	85401-04-3	85401-05-4
85401-06-5	85401-07-6	85401-08-7	85401-09-8	85401-10-1
85401-11-2	85401-13-4	85401-14-5	85401-15-6	85401-16-7
85401-17-8	85401-18-9	85401-19-0	85401-20-3	85401-21-4
85401-22-5	85401-23-6	85401-24-7	85401-25-8	85401-26-9
85401-27-0	85401-28-1	85401-29-2	85401-30-5	85401-31-6
85401-32-7	85401-33-8	85401-34-9	85401-35-0	85401-36-1
85401-37-2	85401-38-3	85401-39-4	85401-40-7	85401-41-8
85401-42-9	85401-43-0	85401-44-1	85401-45-2	85403-34-5
85403-35-6	85403-36-7	85403-37-8	85403-38-9	85403-39-0
85403-40-3	85403-41-4	85403-42-5	85403-43-6	85403-44-7
85403-45-8	85403-46-9	**85403-47-0**	**85403-48-1**	
85403-49-2	85412-35-7	85412-36-8	85412-37-9	85412-38-0
85412-39-1	85412-40-4	85412-73-3	85425-86-1	85425-87-2
85425-88-3	85425-89-4	85425-90-7	85425-91-8	85425-92-9

85425-93-0 85425-94-1
RL: TEM (Technical or engineered material use); USES (Uses)
(dye, for cellulosic textiles)

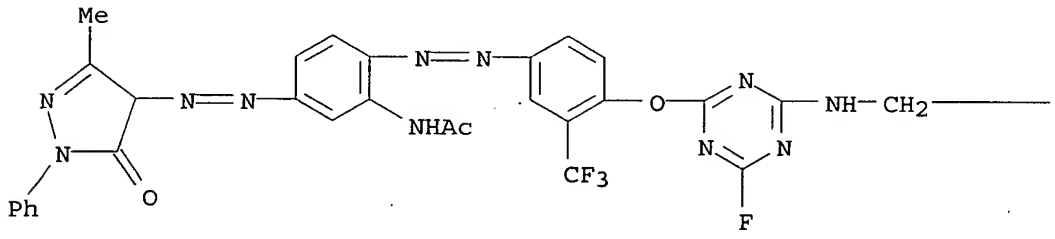
IT **85403-47-0 85403-48-1**
RL: TEM (Technical or engineered material use); USES (Uses)
(dye, for cellulosic textiles)

RN 85403-47-0 HCAPLUS
CN 3H-Pyrazol-3-one, 4-[[4-[[4-[[4-(diethylamino)-6-fluoro-1,3,5-triazin-2-yl]oxy]-3-(trifluoromethyl)phenyl]azo]phenyl]azo]-2,4-dihydro-5-methyl-2-phenyl- (9CI) (CA INDEX NAME)

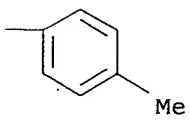


RN 85403-48-1 HCAPLUS
CN Acetamide, N-[5-[(4,5-dihydro-3-methyl-5-oxo-1-phenyl-1H-pyrazol-4-yl)azo]-2-[[4-[[4-fluoro-6-[[(4-methylphenyl)methyl]amino]-1,3,5-triazin-2-yl]oxy]-3-(trifluoromethyl)phenyl]azo]phenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

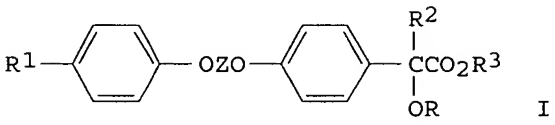


L33 ANSWER 19 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1979:137862 HCAPLUS
DOCUMENT NUMBER: 90:137862

TITLE: 2-Aryloxy-2-(phenoxyalkoxy)phenyl acetic acid and esters
INVENTOR(S): McEvoy, Francis J.; Albright, Jay D.
PATENT ASSIGNEE(S): American Cyanamid Co., USA
SOURCE: U.S., 16 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4125732	A	19781114	US 1977-794510	19770506
ZA 7802041	A	19790328	ZA 1978-2041	19780410
AU 7835157	A1	19791025	AU 1978-35157	19780417
FI 7801298	A	19781107	FI 1978-1298	19780426
NL 7804504	A	19781108	NL 1978-4504	19780426
DE 2819263	A1	19781116	DE 1978-2819263	19780502
BE 866721	A1	19781106	BE 1978-187405	19780505
DK 7801978	A	19781107	DK 1978-1978	19780505
SE 7805185	A	19781107	SE 1978-5185	19780505
FR 2389594	A1	19781201	FR 1978-13417	19780505
FR 2389594	B1	19801031		
DD 136134	C	19790620	DD 1978-205215	19780505
ES 469496	A1	19790916	ES 1978-469496	19780505
HU 19069	O	19801128	HU 1978-AE529	19780505
JP 53137928	A2	19781201	JP 1978-53998	19780506
ES 471826	A1	19791016	ES 1978-471826	19780718

PRIORITY APPLN. INFO.: US 1977-794510 A 19770506
GI



I

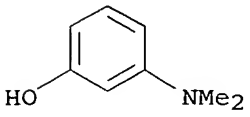
AB Seventy-one hypolipidemic compds. I [R = 3,4- Me2C6H3, 3,4-MeClC6H3, 4,2-Me3CClC6H3, 5-indanyl, 5,6,7,8-tetrahydro-2- naphthyl, 3-, 4-R4C6H3 (R4 = H, Cl, cyano, C1-4 alkyl, CF3, PhO, PhCH2O, cyclohexyl); R1 = F, Cl, CF3, CMe3; R2 = H, C1-6 alkyl; R3 = H, C1-4 alkyl; Z = (CH2)n (n = 1, 2, 3), CHMeCH2, CH2CHMe] and the pharmaceutically acceptable salts of I (R3 = H) were prepared Thus, a mixture of KI, (Me2N)3PO, and 4-ClC6H4OCH2Cl in AcNMe2 was added to NaH and 4-HOC6H4CH2CO2Me in AcNMe2, the product 4-(4-ClC6H4OCH2O)C6H4CH2CO2Me brominated with N-bromosuccinimide, the resulting 4-(4-ClC6H4OCH2O)C6H4CHBrCO2Me etherified with 3,4-Me2C6H4OH and NaH, and the product 4-(4-ClC6H4OCH2O)C6H4CH(OC6H3Me2-3,4)CO2R5 (II, R5 = Me) saponified to give II (R5 = H). At 0.1% in the diet of rats, II (R5 = H) lowered serum sterols 37% and serum triglycerides 64%.
IC C07C065-14
NCL 560062000
CC 28-18 (Heterocyclic Compounds (More Than One Hetero Atom))
IT 59-50-7 95-65-8 98-17-9 98-28-2 98-54-4 **99-07-0**
99-89-8 103-16-2 106-48-9 108-43-0 371-41-5 402-45-9 585-34-2
713-68-8 767-00-0 831-82-3 1131-60-8 1470-94-6
RL: RCT (Reactant); RACT (Reactant or reagent)

(etherification of bromo[(phenoxymethoxy)phenyl]acetates by)

IT **69182-75-8P 69182-85-0P 69182-89-4P**
69182-93-0P 69182-96-3P **69182-97-4P 69183-28-4P**
69183-36-4P 69183-45-5P 69183-49-9P
69183-56-8P 69183-61-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and etherification of, by phenols)

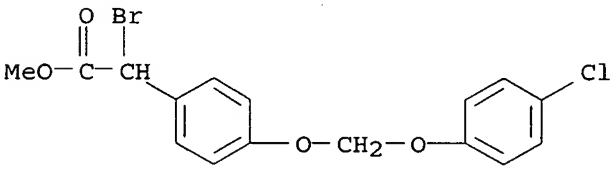
IT **99-07-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(etherification of bromo[(phenoxymethoxy)phenyl]acetates by)

RN 99-07-0 HCAPLUS
CN Phenol, 3-(dimethylamino)- (9CI) (CA INDEX NAME)

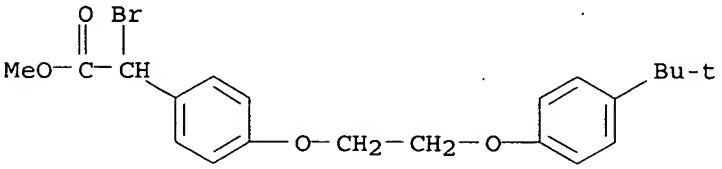


IT **69182-75-8P 69182-85-0P 69182-89-4P**
69182-97-4P 69183-28-4P 69183-36-4P
69183-45-5P 69183-49-9P 69183-56-8P
69183-61-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and etherification of, by phenols)

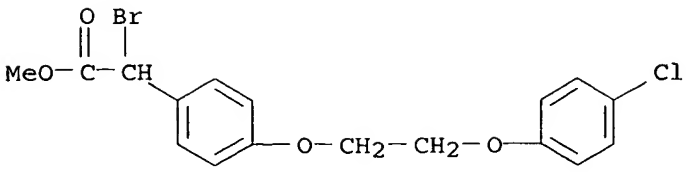
RN 69182-75-8 HCAPLUS
CN Benzeneacetic acid, α-bromo-4-[(4-chlorophenoxy)methoxy]-, methyl ester (9CI) (CA INDEX NAME)



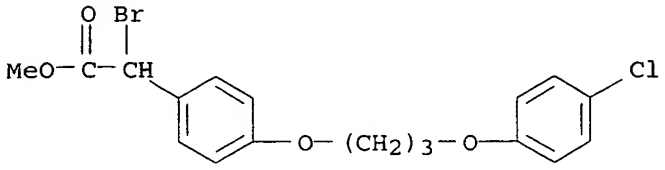
RN 69182-85-0 HCAPLUS
CN Benzeneacetic acid, α-bromo-4-[2-[4-(1,1-dimethylethyl)phenoxy]ethoxy]-, methyl ester (9CI) (CA INDEX NAME)



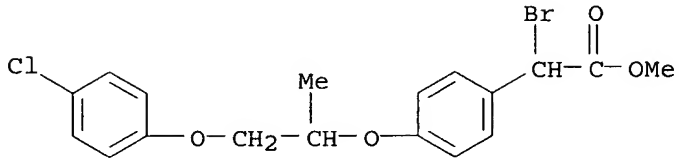
RN 69182-89-4 HCAPLUS
CN Benzeneacetic acid, α-bromo-4-[2-(4-chlorophenoxy)ethoxy]-, methyl ester (9CI) (CA INDEX NAME)



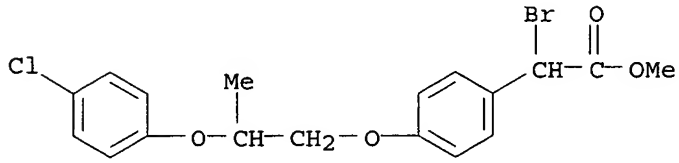
RN 69182-97-4 HCAPLUS
CN Benzeneacetic acid, α-bromo-4-[3-(4-chlorophenoxy)propoxy]-, methyl ester (9CI) (CA INDEX NAME)



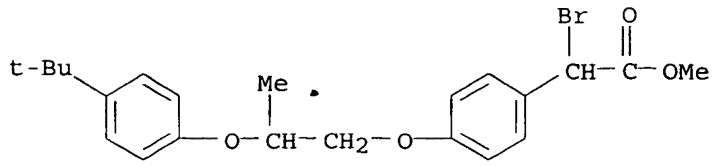
RN 69183-28-4 HCAPLUS
CN Benzeneacetic acid, α-bromo-4-[2-(4-chlorophenoxy)-1-methylethoxy]-, methyl ester (9CI) (CA INDEX NAME)



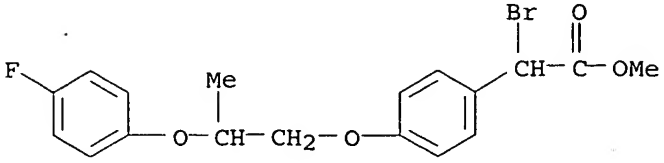
RN 69183-36-4 HCAPLUS
CN Benzeneacetic acid, α-bromo-4-[2-(4-chlorophenoxy)propoxy]-, methyl ester (9CI) (CA INDEX NAME)



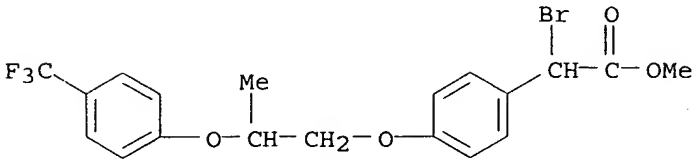
RN 69183-45-5 HCAPLUS
CN Benzeneacetic acid, α-bromo-4-[2-[4-(1,1-dimethylethyl)phenoxy]propoxy]-, methyl ester (9CI) (CA INDEX NAME)



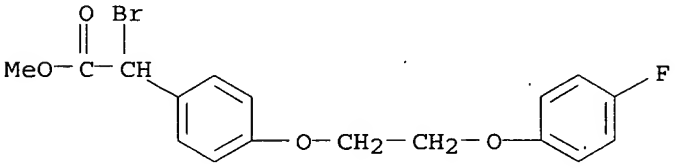
RN 69183-49-9 HCAPLUS
CN Benzeneacetic acid, α-bromo-4-[2-(4-fluorophenoxy)propoxy]-, methyl ester (9CI) (CA INDEX NAME)



RN 69183-56-8 HCAPLUS
CN Benzeneacetic acid, α-bromo-4-[2-[4-(trifluoromethyl)phenoxy]propoxy]-, methyl ester (9CI) (CA INDEX NAME)



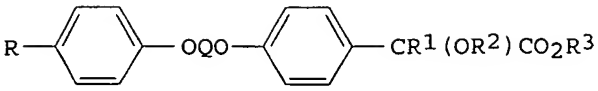
RN 69183-61-5 HCAPLUS
CN Benzeneacetic acid, α-bromo-4-[2-(4-fluorophenoxy)ethoxy]-, methyl ester (9CI) (CA INDEX NAME)



L33 ANSWER 20 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1979:121231 HCAPLUS
DOCUMENT NUMBER: 90:121231
TITLE: Substituted p-phenoxyalkoxyphenylacetic acids and esters of these acids
INVENTOR(S): McEvoy, Francis Joseph; Albright, Jay Donald
PATENT ASSIGNEE(S): American Cyanamid Co., USA
SOURCE: Ger. Offen., 66 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
DE 2819263	A1	19781116	DE 1978-2819263		19780502
US 4125732	A	19781114	US 1977-794510		19770506
PRIORITY APPLN. INFO.:			US 1977-794510	A	19770506

GI



I

AB Hypolipemic title compds. I [R = Cl, F, CF3, CMe3; R1 = H or C1-6 n-alkyl; R2 = substituted Ph, 5-indanyl or 5,6,7,8-tetrahydro-2-naphthyl; R3 = H or C1-4 alkyl; Q = (CH2)1-3, CHMeCH2 or CH2CHMe] were prepared Thus, p-ClC6H4OCH2OCBrPhCO2Me treated with p-Me3CC6H4OH in the presence of NaH and (Me2N)3PO in THF gave I (R = Cl, R1 = H, R2 = p-Me3CC6H4, R3 = Me, Q = CH2), which, at 0.1 weight% in feed to rats, lowered their cholesterol and triglyceride levels in blood serum by 31 and 53%, resp.

IC C07C069-76

CC 25-18 (Noncondensed Aromatic Compounds)

IT 95-65-8 98-54-4 **99-07-0** 106-48-9 402-45-9 585-34-2
1470-94-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with Me bromoacetate)

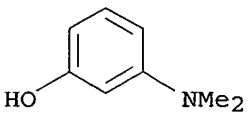
IT **69183-61-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and condensation with phenol)

IT **69182-75-8P 69182-85-0P 69182-89-4P**
69182-93-0P 69182-96-3P **69182-97-4P** 69182-99-6P
69183-02-4P 69183-03-5P 69183-04-6P 69183-06-8P 69183-07-9P
69183-28-4P 69183-36-4P 69183-45-5P
69183-49-9P 69183-56-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and condensation with phenols)

IT **99-07-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with Me bromoacetate)

RN 99-07-0 HCAPLUS

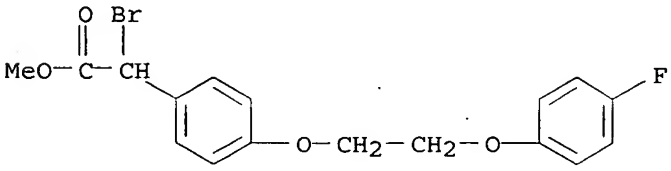
CN Phenol, 3-(dimethylamino)- (9CI) (CA INDEX NAME)



IT **69183-61-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and condensation with phenol)

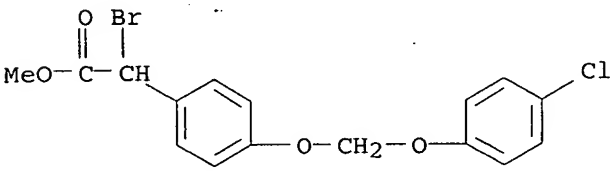
RN 69183-61-5 HCAPLUS

CN Benzeneacetic acid, α-bromo-4-[2-(4-fluorophenoxy)ethoxy]-, methyl ester (9CI) (CA INDEX NAME)

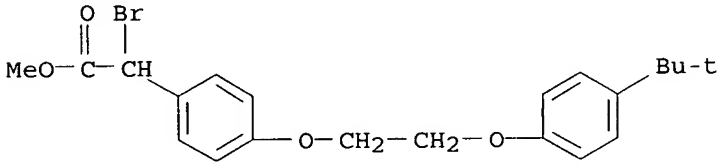


IT **69182-75-8P 69182-85-0P 69182-89-4P**
69182-97-4P 69183-28-4P 69183-36-4P
69183-45-5P 69183-49-9P 69183-56-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and condensation with phenols)

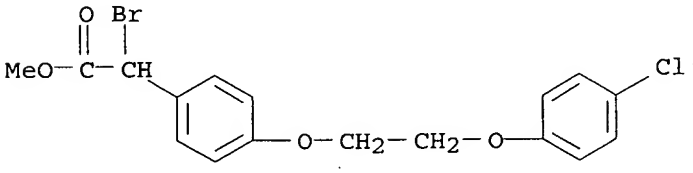
RN 69182-75-8 HCAPLUS
CN Benzeneacetic acid, α-bromo-4-[(4-chlorophenoxy)methoxy]-, methyl ester (9CI) (CA INDEX NAME)



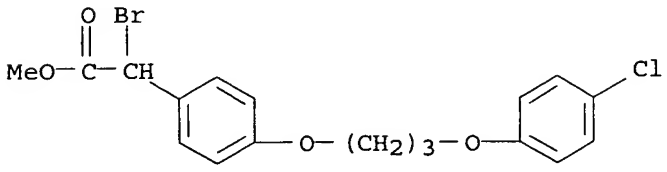
RN 69182-85-0 HCAPLUS
CN Benzeneacetic acid, α-bromo-4-[2-[4-(1,1-dimethylethyl)phenoxy]ethoxy]-, methyl ester (9CI) (CA INDEX NAME)



RN 69182-89-4 HCAPLUS
CN Benzeneacetic acid, α-bromo-4-[2-(4-chlorophenoxy)ethoxy]-, methyl ester (9CI) (CA INDEX NAME)

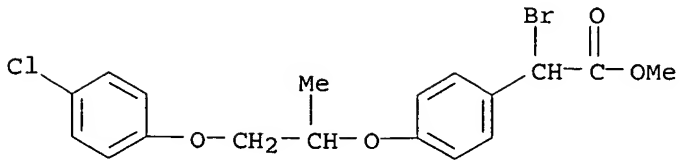


RN 69182-97-4 HCAPLUS
CN Benzeneacetic acid, α-bromo-4-[3-(4-chlorophenoxy)propoxy]-, methyl ester (9CI) (CA INDEX NAME)

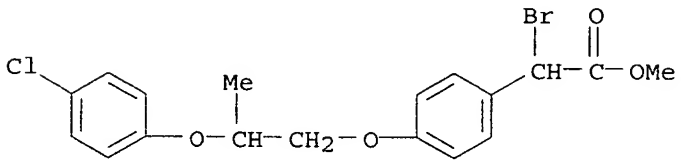


RN 69183-28-4 HCAPLUS
CN Benzeneacetic acid, α-bromo-4-[2-(4-chlorophenoxy)-1-methylethoxy]-,

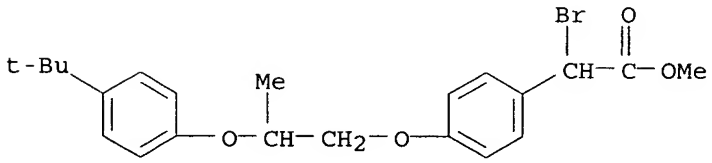
methyl ester (9CI) (CA INDEX NAME)



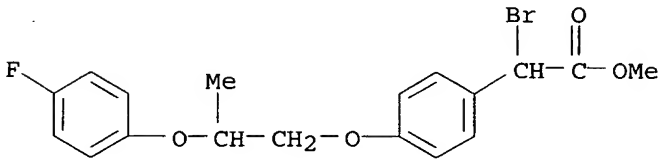
RN 69183-36-4 HCAPLUS
CN Benzeneacetic acid, α-bromo-4-[2-(4-chlorophenoxy)propoxy]-, methyl ester (9CI) (CA INDEX NAME)



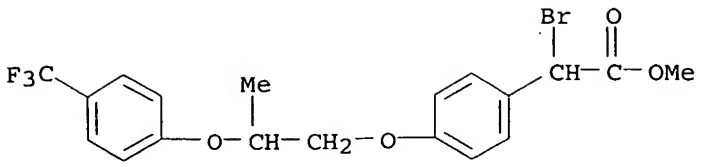
RN 69183-45-5 HCAPLUS
CN Benzeneacetic acid, α-bromo-4-[2-[4-(1,1-dimethylethyl)phenoxy]propoxy]-, methyl ester (9CI) (CA INDEX NAME)



RN 69183-49-9 HCAPLUS
CN Benzeneacetic acid, α-bromo-4-[2-(4-fluorophenoxy)propoxy]-, methyl ester (9CI) (CA INDEX NAME)



RN 69183-56-8 HCAPLUS
CN Benzeneacetic acid, α-bromo-4-[2-[4-(trifluoromethyl)phenoxy]propoxy]-, methyl ester (9CI) (CA INDEX NAME)

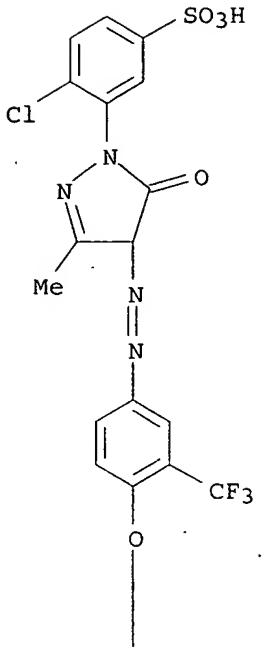


L33 ANSWER 21 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1972:566158 HCAPLUS
DOCUMENT NUMBER: 77:166158
TITLE: Azo dyes for polyamide fibers
INVENTOR(S): Tanaka, Yoshio; Itani, Takashi
PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd.
SOURCE: Jpn. Tokkyo Koho, 6 pp.
CODEN: JAXXAD
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

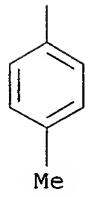
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 47025446	B4	19720711	JP 1969-17032	19690305

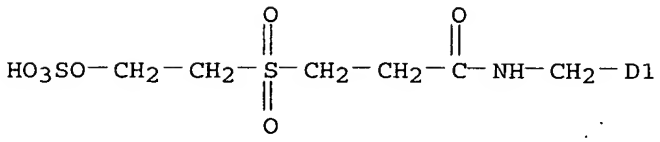
AB Azo dyes (I) were prepared which were used to dye wool and nylon light- and wetfast yellow shades. For example, 4-MeC6H4OC6H3(CF3)NH2-3,4 .far. 1-(2,5-dichloro-4-sulfophenyl)-3-methyl-5-pyrazolone was treated with HOCH2NHCOCH2CH2SO2CH2CH2OH in H2SO4 at 10-15.deg. to give azo dye I(X = Cl; Y = 5-Cl; 4-SO3H; Z = HO; 4-CF3; R = H) [36956-61-3]. Also prepared were I (X = Y = H; 3-SO3H; Z = H2N; 3-CF3; R = Me) and I(X = Cl; Y = H; 5-SO3H; Z = HO; 2-CF3; R = H).
IC C09B
CC 40-4 (Dyes, Fluorescent Whitening Agents, and Photosensitizers)
IT **Dyes, reactive**
([[(sulfooxy)ethyl]sulfonyl][[(trifluoromethyl)phenoxy]benzyl]propanamide **azo** derivs., polyamide and wool fibers)
IT 36956-61-3P 38889-19-9P **38889-20-2P**
RL: IMF (Industrial manufacture); PREP (Preparation)
(preparation of)
IT **38889-20-2P**
RL: IMF (Industrial manufacture); PREP (Preparation)
(preparation of)
RN 38889-20-2 HCAPLUS
CN Benzenesulfonic acid, 4-chloro-3-[4,5-dihydro-3-methyl-4-[[4-[4-methyl[[[1-oxo-3-[[2-(sulfooxy)ethyl]sulfonyl]propyl]amino]methyl]phenoxy]-3-(trifluoromethyl)phenyl]azo]-5-oxo-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A





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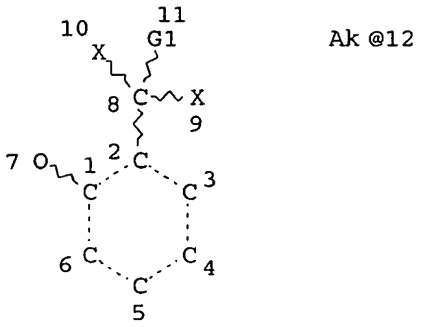

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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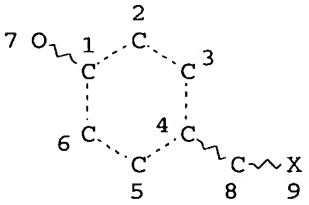

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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE

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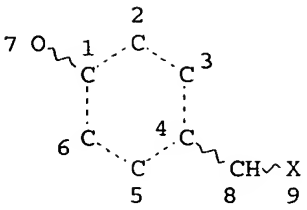


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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   9

STEREO ATTRIBUTES: NONE
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L20         4291 SEA FILE=REGISTRY ABB=ON  PLU=ON  L9 OR L19
L38         3528 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ENZYMES+PFT/CT(L)HYDROL?
L39        27271 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L38 OR HYDROL?(3A)?ENZYME?
L40            4 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L39 AND L20
L41       169861 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ENZYMES+PFT/CT
L42           12 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L20 AND L41
L43           15 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L40 OR L42


=> d l43 ibib abs hitind hitstr 1-15

L43  ANSWER 1 OF 15  HCAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:         2003:656569  HCAPLUS
DOCUMENT NUMBER:          139:191396
TITLE:                    Biphenyl derivatives and their use as antiandrogenic
                          agents
INVENTOR(S):              Labrie, Fernand; Singh, Shankar Mohan; Luu, The Van
PATENT ASSIGNEE(S):       EndoRecherche, Inc., Can.
SOURCE:                   PCT Int. Appl., 58 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.         DATE
     ---------------      ----   --------    --------------------    --------
     WO 2003068217         A1    20030821    WO 2003-CA208           20030214
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ,
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2004006134	A1	20040108	US 2003-369267	20030214
EP 1474127	A1	20041110	EP 2003-702233	20030214

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

PRIORITY APPLN. INFO.:	US 2002-357785P	P 20020215
	WO 2003-CA208	W 20030214

OTHER SOURCE(S): MARPAT 139:191396

AB Biphenyl derivs. are disclosed for use in the treatment of androgen-dependent diseases such as prostate cancer, benign prostatic hyperplasia, precocious puberty, polycystic ovarian syndrome, acne, hirsutism, seborrhea, androgenic alopecia and premature male baldness. For example, some preferred compds. having the structure (formula I): are formulated together with pharmaceutically acceptable diluent or carrier for topical use in the treatment of androgen-dependent prostate cancer.

IC ICM A61K031-277
ICS A61K031-085; A61P005-28; A61P017-10; A61P013-08

CC 1-6 (Pharmacology)
Section cross-reference(s): 63

IT **Enzymes, biological studies**
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(Prostate Short-Chain Dehydrogenase Reductase 1; biphenyl derivs. as antiandrogenic agents)

IT 1591-30-6, [1,1'-Biphenyl]-4,4'-dicarbonitrile 2143-90-0 4854-84-6
10540-31-5 58743-77-4 86111-55-9 **149537-18-8** 582293-04-7
582293-05-8 582293-06-9 582293-07-0 582293-08-1 582293-09-2
582293-10-5 582293-11-6 582293-12-7 582293-13-8 582293-14-9
582293-15-0 582293-16-1 582293-17-2 582293-18-3 582293-20-7
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582293-53-6 582293-54-7 582293-55-8 582293-56-9 582293-57-0
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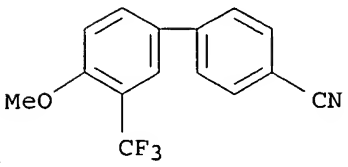
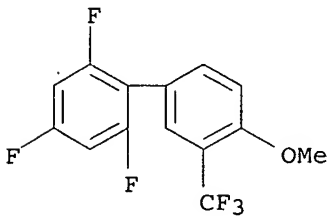
582294-15-3 582294-16-4 582294-17-5 582294-18-6 582294-19-7
582294-38-0
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(biphenyl derivs. as antiandrogenic agents)

IT **149537-18-8 582293-83-2**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(biphenyl derivs. as antiandrogenic agents)

RN 149537-18-8 HCAPLUS
CN [1,1'-Biphenyl]-4-carbonitrile, 4'-methoxy-3'-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 582293-83-2 HCAPLUS
CN 1,1'-Biphenyl, 2,4,6-trifluoro-4'-methoxy-3'-(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L43 ANSWER 2 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:376865 HCAPLUS
DOCUMENT NUMBER: 138:385444
TITLE: Preparation of substituted adenines as drugs, cosmetics, and agrochemical growth regulators.
INVENTOR(S): Dolezal, Karel; Popa, Igor; Holub, Jan; Lenobel, Rene; Werbrouck, Stefaan; Strnad, Miroslav; Zatloukal, Marek
PATENT ASSIGNEE(S): Ustav Experimentalni Botaniky Akademie Ved Ceske Republiky, Czech Rep.
SOURCE: PCT Int. Appl., 67 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003040144	A2	20030515	WO 2002-CZ45	20020801
WO 2003040144	A3	20040226		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,

FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
EP 1419157 A2 20040519 EP 2002-750769 20020801
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK
BR 2002011597 A 20040713 BR 2002-11597 20020801
PRIORITY APPLN. INFO.: CZ 2001-2818 A 20010802
WO 2002-CZ45 W 20020801
OTHER SOURCE(S): MARPAT 138:385444
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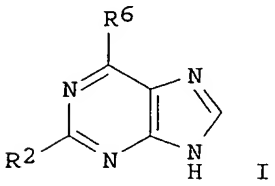


I

AB Title compds. [I; R2 = H, halo, OH, alkoxy, amino, hydrazo, SH, CO2H, cyano, NO2, amido, sulfo, sulfamido, acylamino, acyloxy, cycloalkyl, etc.; R6 = (substituted) alkyl, cycloalkyl, aryl, heterocyclyl, heteroaryl, aralkyl, cycloalkylalkylalkyl, amido, sulfo, etc.], were prepared Thus, 6-chloropurine, 3-chlorobenzylamine, and Et3N were heated in BuOH at 90° for 4 h to give 95% 6-(3-chlorobenzylamino)purine. This showed IC50 = 148.6 μM against G-361 cancer cells.

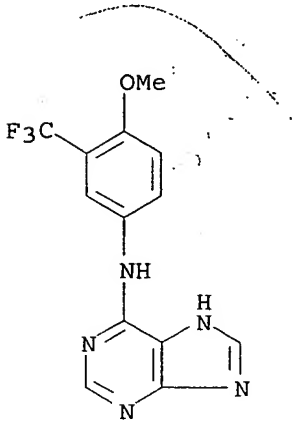
IC ICM C07D473-00
ICS A61K007-00; A61K031-52; A01N043-90; A61P035-00
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 5, 9, 62

IT **Enzymes, uses**
RL: DEV (Device component use); USES (Uses)
(immobilized; preparation of substituted adenines as drugs, cosmetics, and agrochem. growth regulators)

IT 6296-91-9P, 6-(4-Methoxyanilino)purine 6970-39-4P, 6-(3-Methoxyanilino)purine 73663-97-5P, 6-(2-Methoxyanilino)purine 525608-81-5P 525608-82-6P, 6-(3,4-Dichloroanilino)purine 525608-83-7P, 6-(2-Difluoromethoxyanilino)purine 525608-84-8P, 6-[2-Fluoro-4-(trifluoromethyl)anilino]purine 525608-85-9P, 6-(4-Iodo-2-methylanilino)purine 525608-86-0P, 6-(2-Methoxy-5-methylanilino)purine 525608-87-1P, 6-(2-Methoxy-6-methylanilino)purine 525608-88-2P, 6-(4-Methoxy-2-methylanilino)purine 525608-89-3P, 6-(5-Methoxy-2-methylanilino)purine **525608-90-6P**, 6-[4-Methoxy-3-(trifluoromethyl)anilino]purine
RL: AGR (Agricultural use); BSU (Biological study, unclassified); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted adenines as drugs, cosmetics, and agrochem. growth regulators)

IT **525608-90-6P**, 6-[4-Methoxy-3-(trifluoromethyl)anilino]purine
RL: AGR (Agricultural use); BSU (Biological study, unclassified); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted adenines as drugs, cosmetics, and agrochem.

growth regulators)
RN 525608-90-6 HCAPLUS
CN 1H-Purin-6-amine, N-[4-methoxy-3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



L43 ANSWER 3 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:314907 HCAPLUS
DOCUMENT NUMBER: 139:334625
TITLE: Developing a strategy for activity-based detection of enzymes in a protein microarray
AUTHOR(S): Chen, Grace Y. J.; Uttamchandani, Mahesh; Zhu, Qing; Wang, Gang; Yao, Shao Q.
CORPORATE SOURCE: Department of Chemistry, National University of Singapore, Singapore, 117543, Singapore
SOURCE: ChemBioChem (2003), 4(4), 336-339
CODEN: CBCHFX; ISSN: 1439-4227
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The microarray strategy that allows high throughput, activity-based detection of enzymes immobilized on a glass slide, and its potential application for rapid screenings of enzyme inhibitors are described. Three probes (PT-Cy3, VS-Cy3, FP-Cy3) were designed as broad-based probes for the simultaneous identification of class-specific unknown enzymes in a protein microarray. Three major classes of enzymes (phosphatases, cysteine proteases, and serine hydrolases), were chosen as the targets of the study. In addition, a highly specific probe (caspase-1 probe) was also tested and showed high selectivity towards caspase-1 over other noncaspase cysteine proteases. The microarray-based strategy is a protein-array based strategy that allows the detection of proteins not merely by their binding, but rather by their enzymic activities. The strategy may be used as a viable means for rapid assessment of a candidate drug against a large number of its potential target enzymes.
CC 7-1 (Enzymes)
Section cross-reference(s): 6, 9
IT **Enzymes, biological studies**
Proteins
RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)
(strategy for activity-based detection of enzymes in a protein microarray)
IT **615557-60-3** 615557-61-4 615557-62-5 615557-63-6

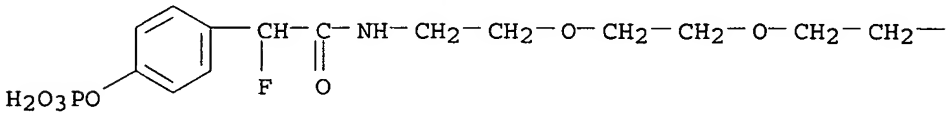
RL: ARG (Analytical reagent use); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(strategy for activity-based detection of enzymes in a protein microarray)

IT **615557-60-3**
RL: ARG (Analytical reagent use); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(strategy for activity-based detection of enzymes in a protein microarray)

RN 615557-60-3 HCAPLUS

CN 3H-Indolium, 2-[3-(1,3-dihydro-1,3,3-trimethyl-2H-indol-2-ylidene)-1-propenyl]-1-[17-fluoro-5,16-dioxo-17-[4-(phosphonooxy)phenyl]-9,12-dioxa-6,15-diazaheptadec-1-yl]-3,3-dimethyl- (9CI) (CA INDEX NAME)

PAGE 1-A



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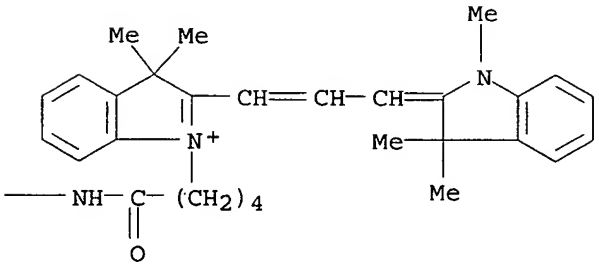


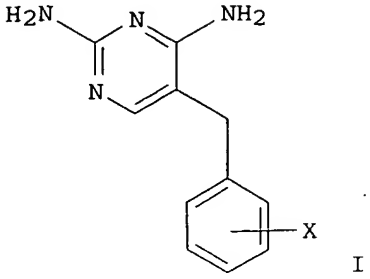
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L43 ANSWER 4 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:326190 HCAPLUS
DOCUMENT NUMBER: 137:232199
TITLE: QSAR for dihydrofolate reductase inhibitors with molecular graph structural descriptors
AUTHOR(S): Ivanciuc, Ovidiu; Ivanciuc, Teodora; Cabrol-Bass, Daniel
CORPORATE SOURCE: Department of Marine Sciences, Texas A & M University at Galveston, Galveston, TX, 77551, USA
SOURCE: THEOCHEM (2002), 582, 39-51
CODEN: THEODJ; ISSN: 0166-1280
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

AB Mol. graph descriptors are used, together with a large diversity of geometric, electrostatic, and quantum indexes, to model phys., chemical, or biol. properties with quant. structure-property relationships and quant. structure-activity relationships of compds. I (X = H, 4-NO2, 3-F, 4-NH2, 4-F, 3-OH, etc). The interest of developing new graph descriptors for organic compds. was stimulated in recent years by their use in virtual screening of combinatorial libraries, database mining, similarity and diversity assessment. Recently, we have extended topol. indexes by defining a series of mol. graph operators, providing an effective systematization and generalization of these structural descriptors. A graph operator uses a math. equation to compute a family of related mol. graph descriptors with different mol. matrixes and various sets of parameters for atoms and bonds. In this paper we use structural descriptors computed with mol. graph operators to develop quant. structure-activity relationships (QSAR) models for the dihydrofolate reductase inhibition with diaminopyrimidines. The mol. descriptors are derived from five mol. matrixes, namely adjacency A, distance D, reciprocal distance RD, distance-path Dp, and reciprocal distance-path RDp. The QSAR models are obtained by selecting descriptors with a genetic algorithm, and the best models are validated with the leave-one-out cross-validation method. The QSAR models with the highest prediction power are comparable with those obtained with substituent consts. and neural networks, but they use a much lower number of parameters.

CC 22-2 (Physical Organic Chemistry)
Section cross-reference(s): 1, 7

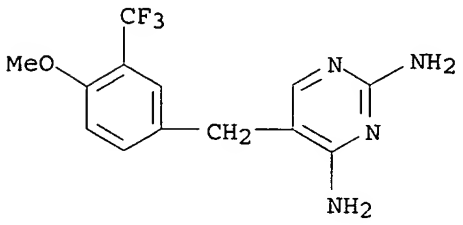
IT **Enzymes, properties**
RL: PRP (Properties)
(inhibitors; QSAR for dihydrofolate reductase inhibitors with mol. graph structural descriptors)

IT 738-70-5 836-06-6 5355-16-8 7319-45-1 13932-40-6 18588-43-7
20285-70-5 20344-69-8 30077-60-2 30077-67-9 36821-85-9
46726-70-9 49561-94-6 49873-11-2 50823-94-4 **50823-96-6**
53808-87-0 56066-63-8 56518-41-3 59481-28-6 68902-57-8
69194-91-8 69945-50-2 69945-51-3 69945-52-4 69945-53-5
69945-54-6 69945-55-7 69945-56-8 69945-57-9 69945-58-0
69945-59-1 69945-60-4 71525-05-8 73090-70-7 73356-40-8
73356-41-9 77113-54-3 77113-55-4 77113-56-5 77113-57-6
77113-58-7 77113-59-8 77113-60-1 77113-61-2 77113-62-3
77113-63-4 78025-72-6 78233-99-5 80407-58-5 80407-59-6
80407-60-9 80407-61-0 80407-62-1 80416-29-1 83158-06-9
83166-76-1 93317-64-7 98612-08-9 98612-09-0 100515-03-5
100515-04-6 107697-99-4 107698-00-0 107698-01-1 107698-02-2

107698-03-3 107698-04-4
RL: PRP (Properties)
(QSAR for dihydrofolate reductase inhibitors with mol. graph structural descriptors)

IT **50823-96-6**
RL: PRP (Properties)
(QSAR for dihydrofolate reductase inhibitors with mol. graph structural descriptors)

RN 50823-96-6 HCAPLUS
CN 2,4-Pyrimidinediamine, 5-[[4-methoxy-3-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L43 ANSWER 5 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:645635 HCAPLUS
DOCUMENT NUMBER: 135:225942
TITLE: Methods and compositions for synthesis of oligosaccharides using mutant glycosidase enzymes
INVENTOR(S): Withers, Stephen G.; MacKenzie, Lloyd; Wang, Qingping
PATENT ASSIGNEE(S): The University of British Columbia, Can.
SOURCE: U.S., 17 pp., Cont.-in-part of U.S. 5,716,812.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6284494	B1	20010904	US 1998-91272	19980929
US 5716812	A	19980210	US 1995-571175	19951212
WO 9721822	A2	19970619	WO 1996-CA841	19961212
WO 9721822	A3	19970828		
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 2003100749	A1	20030529	US 2001-837711	20010417

PRIORITY APPLN. INFO.:

US 1995-571175	A2	19951212
WO 1996-CA841	W	19961212
CA 1995-2165041	A	19951212
US 1998-91272	A1	19980929

OTHER SOURCE(S): CASREACT 135:225942

AB Mutant glycosidase enzymes are formed in which the normal nucleophilic amino acid within the active site has been changed to a non-nucleophilic amino acid. These **enzymes** cannot **hydrolyze** disaccharide products, but can still form them. Using this enzyme, oligosaccharides are synthesized by preparing a mixture of an α-glycosyl fluoride and a glycoside acceptor mol.; enzymically coupling the α-glycosyl fluoride to the glycoside acceptor mol. to form a glycosyl glycoside product using the mutant glycosidase enzyme; and recovering the glycosyl glycoside product. Particular enzymes include a mutant form of Agrobacterium β-glucosidase in which the normal glutamic acid residue at position 358 is replaced with an alanine residue.

IC ICM C12P019-44
ICS C12P019-12; C12N009-24; C12N009-26; C12N009-42

NCL 435074000

CC 16-2 (Fermentation and Bioindustrial Chemistry)
Section cross-reference(s): 7

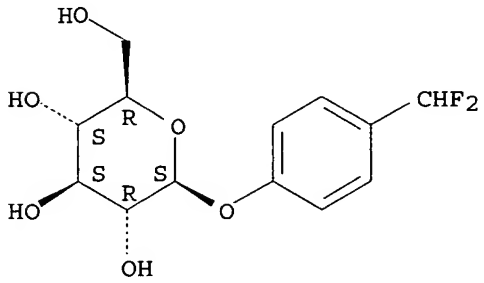
IT 487-60-5 490-51-7 1226-39-7 1464-44-4 2001-96-9 2021-84-3, α-D-Galactopyranosyl fluoride 2106-10-7, α-D-Glucopyranosyl fluoride 2492-87-7, β-D-Glucopyranoside, 4-nitrophenyl 2816-24-2, β-D-Glucopyranoside, 2-nitrophenyl 2936-70-1, β-D-Glucopyranoside, phenyl 1-thio- 3150-24-1, β-D-Galactopyranoside, 4-nitrophenyl 3482-57-3 4304-12-5 6032-32-2, β-D-Glucopyranoside, 4-methoxyphenyl 7791-61-9 10019-60-0 10238-27-4 17400-77-0 18997-57-4 18997-57-4 20838-44-2 25775-97-7, β-D-Glucopyranoside, 2,4-dinitrophenyl 35599-02-1 62499-26-7 70569-27-6 75705-24-7, Benzoic acid, 4-(β-D-glucopyranosyloxy)-, methyl ester 111495-86-4 **131497-36-4** 168291-98-3 188194-13-0 192657-49-1 192657-50-4 358395-47-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of oligosaccharides using mutant glycosidase enzymes)

IT **131497-36-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of oligosaccharides using mutant glycosidase enzymes)

RN 131497-36-4 HCAPLUS

CN β-D-Glucopyranoside, 4-(difluoromethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L43 ANSWER 6 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:152525 HCAPLUS

DOCUMENT NUMBER: 134:212695

TITLE: Drug conjugates comprising vector-linker-pharmacophore and methods of designing the same

INVENTOR(S): Brenner, Sydney; Goelet, Philip; Stackhouse, Joseph; Millward, Steven W.
PATENT ASSIGNEE(S): USA
SOURCE: PCT Int. Appl., 196 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001013958	A2	20010301	WO 2000-US23593	20000828
WO 2001013958	A3	20020131		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2382202	AA	20010301	CA 2000-2382202	20000828
EP 1212096	A2	20020612	EP 2000-959512	20000828
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003507439	T2	20030225	JP 2001-518093	20000828

PRIORITY APPLN. INFO.:

US 1999-150765P	P	19990826
US 1999-150894P	P	19990826
US 2000-184411P	P	20000223
US 2000-184412P	P	20000223
WO 2000-US23593	W	20000828

AB The invention relates to drug conjugates and methods of their design. One embodiment of the invention is directed to a method of designing vector-linker-pharmacophore (VLP) conjugates that is generally applicable to a wide variety of vectors, linkers, and pharmacophores. The invention also encompasses a method of improving the delivery of a pharmacophore to a patient, as well as a method of improving the therapeutic efficacy of a pharmacophore and a method of decreasing the toxicity of a pharmacophore. A method of increasing the concentration of a pharmacophore in a cell is further encompassed by the invention. Preparation of many VLP conjugates including conjugates of kirromycin-3-nitro-4-hydrazidophenylthioethanol-tetracycline derivative, are disclosed.

IC ICM A61K047-48
CC 63-5 (Pharmaceuticals)
Section cross-reference(s): 28
IT **Enzymes, biological studies**
Proteins, general, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(inhibitors; drug conjugates comprising vector-linker-pharmacophore and methods of designing same)
IT 104-10-9P 107-68-6P, N-Methyltaurine 501-53-1P, Carbobenzyloxy chloride 1007-54-1P 3163-15-3P, 2-Aminoresorcinol 5063-96-7P 6066-83-7P, 5-Aminovaleronitrile 15896-61-4P 17385-61-4P 19285-38-2P 21253-57-6P 21253-58-7P 21822-24-2P 52648-14-3P, 1-N-Desmethylgoldinamine 73164-56-4P 74219-55-9P 86386-77-8P 116435-82-6P 120793-45-5P 143429-10-1P 155834-18-7P 161321-16-0P

161321-34-2P 188434-24-4P **188434-25-5P 188434-26-6P**
328400-43-7P 328400-46-0P 328400-48-2P 328400-50-6P 328400-52-8P
328400-54-0P 328400-56-2P 328400-60-8P 328400-62-0P 328400-64-2P
328400-66-4P 328400-68-6P 328400-71-1P 328400-73-3P 328400-75-5P
328400-77-7P 328400-79-9P 328400-81-3P 328400-83-5P 328400-87-9P
328400-89-1P 328400-91-5P 328400-93-7P 328400-95-9P 328400-98-2P
328401-02-1P 328401-08-7P 328401-09-8P 328401-10-1P 328401-11-2P
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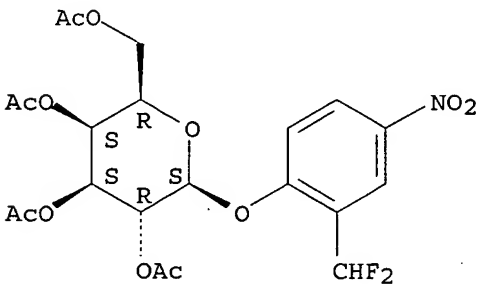
328401-51-0P 328401-53-2P 328401-54-3P 328401-55-4P 328401-57-6P
328401-59-8P 328401-61-2P 328401-63-4P 328401-64-5P 328401-66-7P
328401-68-9P 328401-69-0DP, derivs. 328401-71-4P 328401-72-5P
328401-73-6P 328401-74-7P 328401-75-8P 328401-76-9P 328401-77-0P
328899-82-7P, Goldinonic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(drug conjugates comprising vector-linker-pharmacophore and methods of designing same)

IT **188434-25-5P 188434-26-6P 328401-17-8P**
328401-18-9P 328401-19-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(drug conjugates comprising vector-linker-pharmacophore and methods of designing same)

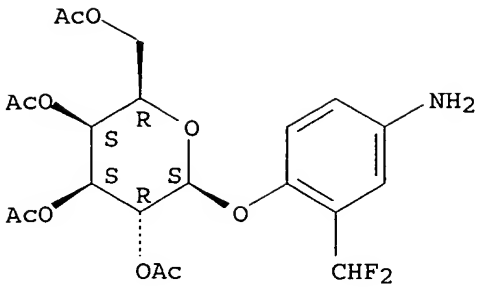
RN 188434-25-5 HCAPLUS
CN β-D-Galactopyranoside, 2-(difluoromethyl)-4-nitrophenyl, 2,3,4,6-tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



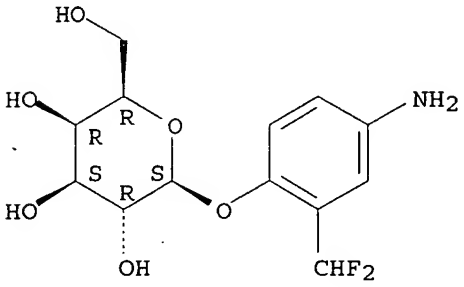
RN 188434-26-6 HCAPLUS
CN β-D-Galactopyranoside, 4-amino-2-(difluoromethyl)phenyl, 2,3,4,6-tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



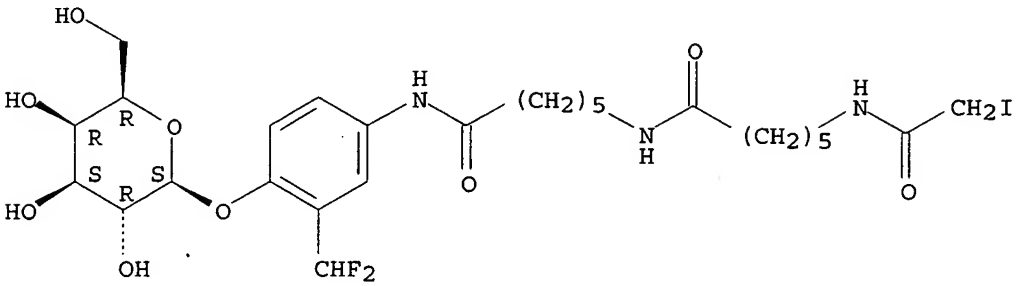
RN 328401-17-8 HCAPLUS
CN β-D-Galactopyranoside, 4-amino-2-(difluoromethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



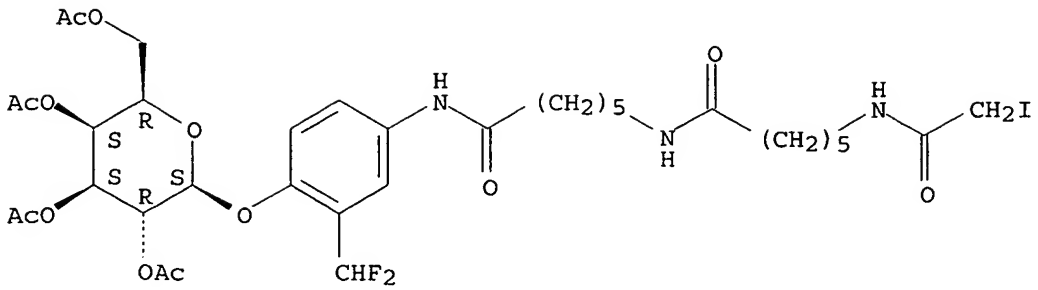
RN 328401-18-9 HCAPLUS
CN Hexanamide, N-[6-[[3-(difluoromethyl)-4-(β-D-galactopyranosyloxy)phenyl]amino]-6-oxohexyl]-6-[(iodoacetyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

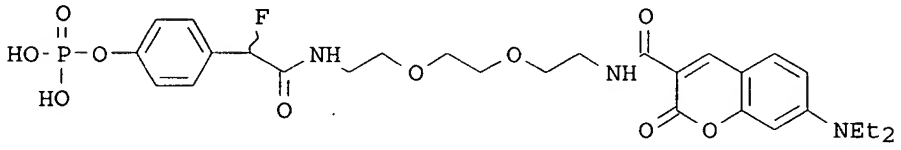


RN 328401-19-0 HCAPLUS
CN Hexanamide, N-[6-[[3-(difluoromethyl)-4-[(2,3,4,6-tetra-O-acetyl-β-D-galactopyranosyl)oxy]phenyl]amino]-6-oxohexyl]-6-[(iodoacetyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L43 ANSWER 7 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:693502 HCAPLUS
DOCUMENT NUMBER: 132:35824
TITLE: Design and synthesis of an activity probe for protein tyrosine phosphatases
AUTHOR(S): Lo, Lee-Chiang; Wang, Hsin-Yi; Wang, Zi-Jien
CORPORATE SOURCE: Department of Chemistry, National Taiwan University, Taipei, 106, Taiwan
SOURCE: Journal of the Chinese Chemical Society (Taipei) (1999), 46(5), 715-718
CODEN: JCCTAC; ISSN: 0009-4536
PUBLISHER: Chinese Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB Protein tyrosine phosphatases (PTPases) are an important class of enzymes involved in the regulation of many cellular events. The design and synthesis of an activity probe I targeting these PTPases is described. This mechanism-based activity probe adopts a cassette-like design; a phosphate group serves as the recognition head and a fluorescent diethylaminocoumarin derivative acts as the reporter group. Compound 4-HOC6H4CHOHCONHCH2CH2OCH2CH2OCH2CH2NHCO2CMe3 was phosphorylated with diallyl phosphorochloridate and then fluorinated with DAST to give versatile intermediate. The Boc protective group of compound intermediate was removed by TFA to make available the amino group where a diethylaminocoumarin chromophore was later attached. Final deprotection of the allyl group from the phosphate head gives complete activity probe I. It will be used in the labeling study of PTPases from various sources.

CC 29-7 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 1

IT **Enzymes, biological studies**
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL

(Biological study); PROC (Process)
(protein tyrosine phosphatases; design and synthesis of activity probe for protein tyrosine phosphatases)

IT **252259-74-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(design and synthesis of activity probe for protein tyrosine phosphatases)

IT **252259-76-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and amine deprotection of)

IT **252259-79-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deallylation of)

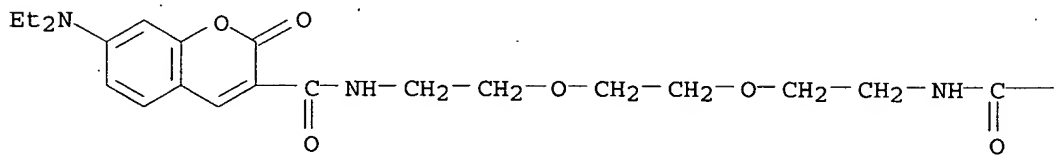
IT **252259-78-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with diethylaminocoumarin chromophore)

IT **252259-74-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(design and synthesis of activity probe for protein tyrosine phosphatases)

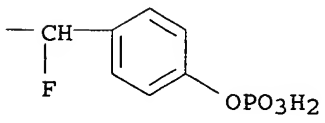
RN 252259-74-8 HCAPLUS

CN 2H-1-Benzopyran-3-carboxamide, 7-(diethylamino)-N-[2-[2-[2-[[fluoro[4-(phosphonooxy)phenyl]acetyl]amino]ethoxy]ethoxy]ethyl]-2-oxo- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



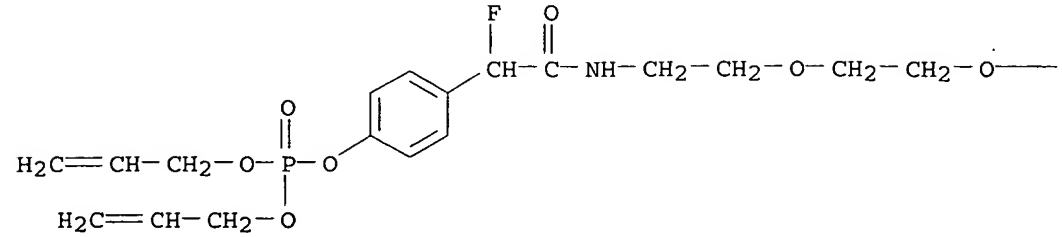
IT **252259-76-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and amine deprotection of)

RN 252259-76-0 HCAPLUS

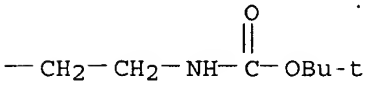
CN 5,8-Dioxa-2,11-diazatridecanoic acid, 13-[4-[[bis(2-

propenyloxy)phosphinyl]oxy]phenyl]-13-fluoro-12-oxo-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

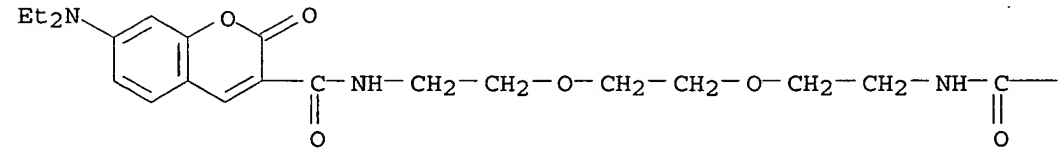


PAGE 1-B

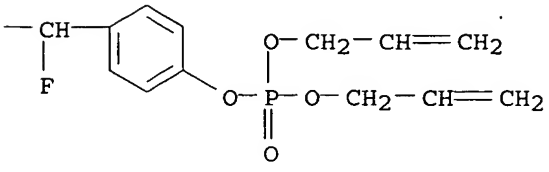


IT **252259-79-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deallylation of)
RN 252259-79-3 HCAPLUS
CN Phosphoric acid, 4-[13-[7-(diethylamino)-2-oxo-2H-1-benzopyran-3-yl]-1-fluoro-2,13-dioxo-6,9-dioxa-3,12-diazatridec-1-yl]phenyl di-2-propenyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



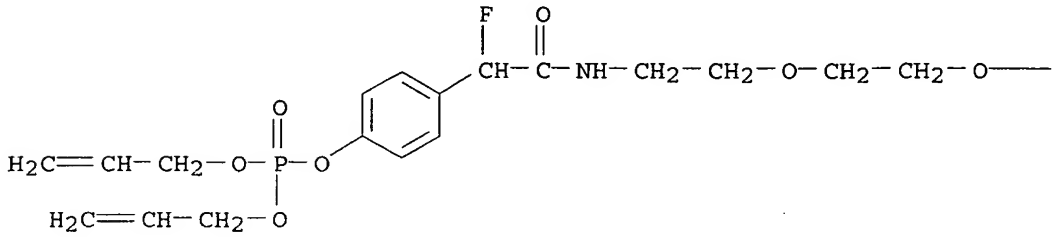
IT **252259-78-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with diethylaminocoumarin chromophore)

RN 252259-78-2 HCAPLUS
CN Phosphoric acid, 4-[2-[[2-[2-(2-aminoethoxy)ethoxy]ethyl]amino]-1-fluoro-2-oxoethyl]phenyl di-2-propenyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 252259-77-1
CMF C20 H30 F N2 O7 P

PAGE 1-A



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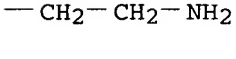
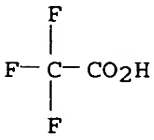


CM 2

CRN 76-05-1
CMF C2 H F3 O2



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L43 ANSWER 8 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:793124 HCAPLUS
DOCUMENT NUMBER: 130:37298
TITLE: Conjugates and specific immunoassays for methadone metabolite 2-ethylidine-1,5-dimethyl-3,3-diphenylpyrrolidine
INVENTOR(S): Sigler, Gerald Francis; Coty, William; Powell, Michael Joseph
PATENT ASSIGNEE(S): Boehringer Mannheim Corporation, USA
SOURCE: PCT Int. Appl., 55 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9854133	A1	19981203	WO 1997-US17784	19970924
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2259898	AA	19981203	CA 1997-2259898	19970924
AU 9748938	A1	19981230	AU 1997-48938	19970924
EP 931062	A1	19990728	EP 1997-911614	19970924
EP 931062	B1	20041117		
R: CH, DE, ES, FR, GB, IT, LI, NL				
US 6140137	A	20001031	US 1998-930959	19980924
PRIORITY APPLN. INFO.:			US 1997-47773P P	19970527
			WO 1997-US17784 W	19970924

OTHER SOURCE(S): MARPAT 130:37298

AB Novel chemical analogs of the methadone metabolite 2-ethylidene-1,5-dimethyl-3,3-diphenylpyrrolidine (EDDP) are disclosed. The derivs. can be used for formation of EDDP-protein conjugates. The conjugates can be used in turn to raise antibodies reactive with EDDP and having a low cross-reactivity with methadone. The antibodies and EDDP-enzyme polypeptide conjugates provide the basis for specific immunoassays used in monitoring compliance with methadone treatment (for withdrawal from heroin addiction).

IC ICM C07D207-20
ICS G01N033-94

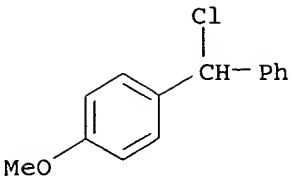
CC 15-2 (Immunochemistry)
Section cross-reference(s): 1, 4

IT **Enzymes, biological studies**
Proteins, specific or class
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(conjugates, EDDP analogs; preparation of hapten conjugates of EDDP analogs for raising antibody for immunoassay of methadon metabolites and for monitoring methadone treatment for withdrawal from heroin addiction)

IT 720-44-5P 4578-79-4P **6731-11-9P**, p-Methoxybenzhydryl chloride
104357-17-7P 216974-53-7P 216974-56-0P 216974-59-3P 216974-64-0P
216974-66-2P 216974-68-4P 216974-69-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of hapten conjugates of EDDP analogs for raising antibody for immunoassay of methadon metabolites and for monitoring methadone treatment for withdrawal from heroin addiction)

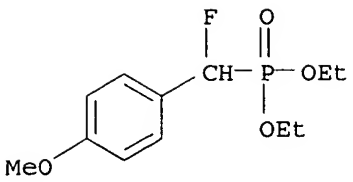
IT **6731-11-9P**, p-Methoxybenzhydryl chloride
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of hapten conjugates of EDDP analogs for raising antibody for immunoassay of methadon metabolites and for monitoring methadone treatment for withdrawal from heroin addiction)

RN 6731-11-9 HCAPLUS
CN Benzene, 1-(chlorophenylmethyl)-4-methoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L43 ANSWER 9 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:551387 HCAPLUS
DOCUMENT NUMBER: 129:241683
TITLE: Inhibitors directed towards the binuclear metal center of phosphotriesterase. [Erratum to document cited in CA127:274562]
AUTHOR(S): Hong, Suk Bong; Raushel, Frank M.
CORPORATE SOURCE: Dep. Chem., Texas A & M Univ., College Station, TX, 77843, USA
SOURCE: Journal of Enzyme Inhibition (1998), 13(1), No pp. Given
CODEN: ENINEG; ISSN: 8755-5093
PUBLISHER: Harwood Academic Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Structures VI and VII in Table I have been corrected
CC 7-3 (Enzymes)
IT **Enzymes, biological studies**
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(metallo-; inhibitors directed towards the binuclear metal center of phosphotriesterase (Erratum))
IT 78-40-0 298-06-6 598-02-7 683-08-9 884-90-2 1067-71-6 1478-53-1 1663-55-4 1754-49-0 1776-87-0 2609-49-6 3084-40-0 3095-95-2 3453-00-7 6629-49-8 16497-99-7 49640-96-2 56183-69-8 63542-12-1 67964-17-4 70269-57-7 70660-05-8 174349-94-1 177284-54-7 **196514-50-8** 196514-51-9 213077-24-8
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(inhibitors directed towards the binuclear metal center of phosphotriesterase (Erratum))
IT **196514-50-8**
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(inhibitors directed towards the binuclear metal center of phosphotriesterase (Erratum))
RN 196514-50-8 HCAPLUS
CN Phosphonic acid, [fluoro(4-methoxyphenyl)methyl]-, diethyl ester (9CI) (CA INDEX NAME)



L43 ANSWER 10 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:597993 HCAPLUS
DOCUMENT NUMBER: 127:274562
TITLE: Inhibitors directed towards the binuclear metal center of phosphotriesterase
AUTHOR(S): Hong, Suk Bong; Raushel, Frank M.
CORPORATE SOURCE: Dep. Chem., Texas A & M Univ., College Station, TX, 77843, USA
SOURCE: Journal of Enzyme Inhibition (1997), 12(3), 191-203
CODEN: ENINEG; ISSN: 8755-5093
PUBLISHER: Harwood
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The potential roles in binding and catalysis for the binuclear metal center found within bacterial phosphotriesterase were evaluated by characterization of the inhibitory properties of 26 substrate and product mimetics. Phosphonates bearing monofluoro, difluoro, or hydroxyl substituents at the methylene position were noncompetitive inhibitors with Ki values ranging from 0.6-9 mM vs. the substrate paraoxon. Phosphoramidates did not inhibit the enzyme. Di-Et phosphate and di-Et dithiophosphate inhibited the Cd-substituted enzyme with Ki values of 10 and 130 μM, resp. The most effective inhibitor for either the Cd or Zn substituted enzyme was found di-Et thiomethyl-phosphonate. The competitive inhibition consts. for this compound were 60 nM and 2.8 μM for the Cd- and Zn-substituted enzyme, resp. The tight binding is attributed to chelation of both metal ions simultaneously.

CC 7-3 (Enzymes)

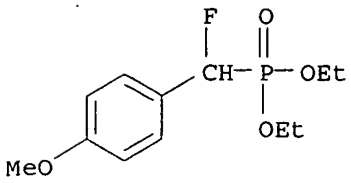
IT **Enzymes, biological studies**
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(metallo-; inhibitors directed towards the binuclear metal center of phosphotriesterase)

IT 78-40-0 298-06-6 598-02-7 683-08-9 884-90-2 1067-71-6 1478-53-1 1754-49-0 1776-87-0 2609-49-6 3084-40-0 3095-95-2 3453-00-7 6629-49-8 16497-99-7 49640-96-2 56183-69-8 63542-12-1 67964-17-4 70269-57-7 70660-05-8 174349-94-1 177284-54-7 **196514-50-8** 196514-51-9
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(inhibitors directed towards the binuclear metal center of phosphotriesterase)

IT **196514-50-8**
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(inhibitors directed towards the binuclear metal center of phosphotriesterase)

RN 196514-50-8 HCAPLUS

CN Phosphonic acid, [fluoro(4-methoxyphenyl)methyl]-, diethyl ester (9CI) (CA INDEX NAME)



L43 ANSWER 11 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:516090 HCAPLUS
DOCUMENT NUMBER: 127:132736
TITLE: Methods and compositions for synthesis of oligosaccharides using mutant glycosidase enzymes
INVENTOR(S): Withers, Stephen G.; Mackenzie, Lloyd; Wang, Quingping
PATENT ASSIGNEE(S): The University of British Columbia, Can.; Withers, Stephen G.; Mackenzie, Lloyd; Wang, Quingping
SOURCE: PCT Int. Appl., 45 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9721822	A2	19970619	WO 1996-CA841	19961212
WO 9721822	A3	19970828		
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2165041	AA	19970613	CA 1995-2165041	19951212
US 5716812	A	19980210	US 1995-571175	19951212
CA 2238966	AA	19970619	CA 1996-2238966	19961212
AU 9711354	A1	19970703	AU 1997-11354	19961212
AU 722220	B2	20000727		
EP 870037	A2	19981014	EP 1996-942211	19961212
EP 870037	B1	20020717		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2000501607	T2	20000215	JP 1997-521572	19961212
EP 1211320	A2	20020605	EP 2001-130513	19961212
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, AL				
AT 220720	E	20020815	AT 1996-942211	19961212
US 6284494	B1	20010904	US 1998-91272	19980929
US 2003100749	A1	20030529	US 2001-837711	20010417

PRIORITY APPLN. INFO.:

CA 1995-2165041	A	19951212
US 1995-571175	A2	19951212
EP 1996-942211	A3	19961212

WO 1996-CA841 W 19961212
US 1998-91272 A1 19980929

AB Mutant glycosidase enzymes are formed in which the normal nucleophilic amino acid within the active site has been changed to a non-nucleophilic amino acid. These **enzymes** cannot **hydrolyze** disaccharide products, but which can still form them. Using this enzyme, oligosaccharides are synthesized by preparing a mixture of an α-glycosyl fluoride and a glycoside acceptor mol., enzymically coupling the α-glycosyl fluoride to the glycoside acceptor mol. to form a glycosyl glycoside product using the mutant glycosidase enzyme, and recovering the glycosyl glycoside product. Particular enzymes include a mutant form of Agrobacterium β-glucosidase in which the normal glutamic acid residue at position 358 is replaced with an alanine residue by using oligonucleotide-directed mutagenesis. Agrobacterium E358A β-glucosidase catalyzed the reaction of α-galactosyl fluoride with p-nitrophenyl-β-D-glucoside to form p-nitrophenyl-4-O-glucopyranosyl-β-D-galactopyranoside in 84% yield. The nature of the donor moiety in some aryl glycosides shifts the reaction from β-1,4 linkages to the production of β-1,3 linkages, but still produces a good yield of product.

IC ICM C12N015-56
ICS C12P019-04; C12N009-24; C12N009-26; C12N015-62

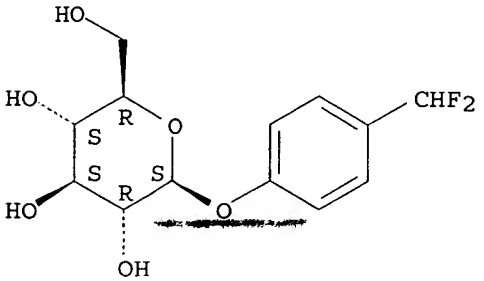
CC 7-3 (Enzymes)
Section cross-reference(s): 9

IT 487-60-5 490-51-7 528-50-7 1226-39-7 1464-44-4, Phenyl β-D-glucoside 2001-96-9 2021-84-3, α-D-Galactosyl fluoride 2106-10-7, α-D-Glucosyl fluoride 2492-87-7, p-Nitrophenyl β-D-glucoside 2816-24-2, 2-Nitrophenyl β-D-glucoside 2936-70-1 3150-24-1 3482-57-3 4304-12-5 6032-32-2 7791-61-9 10238-27-4 18997-57-4 20838-44-2 25775-97-7, β-D-Glucopyranoside, 2,4-dinitrophenyl 35599-02-1 68636-48-6 70569-27-6 75705-24-7 111495-86-4 **131497-36-4** 168291-98-3 188194-13-0 192657-49-1 192657-50-4
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(methods and compns. for synthesis of oligosaccharides using mutant glycosidase enzymes)

IT **131497-36-4**
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(methods and compns. for synthesis of oligosaccharides using mutant glycosidase enzymes)

RN 131497-36-4 HCAPLUS
CN β-D-Glucopyranoside, 4-(difluoromethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L43 ANSWER 12 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:573177 HCAPLUS
DOCUMENT NUMBER: 125:241578
TITLE: A versatile mechanism based reaction probe for the direct selection of biocatalysts
AUTHOR(S): Lo, Lee-Chiang; Lo, Chih-Hung L.; Janda, Kim D.
CORPORATE SOURCE: Deps. Chem. Molecular Biol., Scripps Res. Inst., La Jolla, CA, 92037, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (1996), 6(17), 2117-2120
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A mechanism based reaction probe was synthesized and shown to modify a bacterial phosphotriesterase; this strategy for generating a probe is general and should allow the isolation of a host of unique catalysts.

CC 7-3 (Enzymes)
Section cross-reference(s): 9

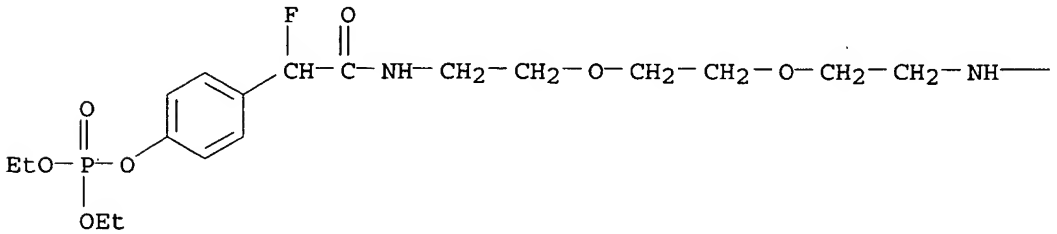
IT **Enzymes**
RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(derivs.; versatile mechanism based reaction probe for direct selection of biocatalysts)

IT **182227-47-0P**
RL: BUU (Biological use, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(versatile mechanism based reaction probe for direct selection of biocatalysts)

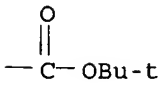
IT **182227-47-0P**
RL: BUU (Biological use, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(versatile mechanism based reaction probe for direct selection of biocatalysts)

RN 182227-47-0 HCAPLUS
CN 5,8-Dioxa-2,11-diazatridecanoic acid, 13-[4-[(diethoxyphosphinyl)oxy]phenyl]-13-fluoro-12-oxo-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



L43 ANSWER 13 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:228471 HCAPLUS
DOCUMENT NUMBER: 122:122490
TITLE: Prodrugs of anthracyclines for chemotherapy via enzyme-monoclonal antibody conjugates
AUTHOR(S): Gesson, J.-P.; Jacquesy, J.-C.; Mondon, M.; Petit, P.; Renoux, B.; Andrianomenjanahary, S.; Van, H. Dufat-Trinh; Koch, M.; Michel, S.; et al.
CORPORATE SOURCE: Lab. Chim. XII, Poitiers, 86022, Fr.
SOURCE: Anti-Cancer Drug Design (1994), 9(5), 409-23
CODEN: ACDDEA; ISSN: 0266-9536
PUBLISHER: Oxford University Press
DOCUMENT TYPE: Journal
LANGUAGE: English

AB New prodrugs of daunorubicin, 1c, 1e and 2c, including a galactopyranosyl residue linked to the N-3' of the daunosaminyl moiety through substituted o- or p-benzyloxycarbonyl groups were synthesized. Their low cytotoxicity and high stability in plasma fulfil the conditions for antibody-directed enzyme prodrug therapy. Enzymic hydrolysis using α-D-galactosidase gives rise to daunorubicin by subsequent self-elimination of the spacers. However, elimination clearly depends on the aromatic substitution pattern, as demonstrated especially by comparison with non-substituted analogs.

CC 1-3 (Pharmacology)
Section cross-reference(s): 26, 63

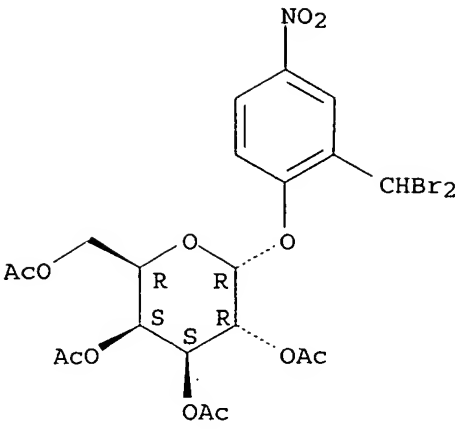
IT **Enzymes**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(prodrugs of anthracyclines for chemotherapy via enzyme-monoclonal antibody conjugates)

IT 52730-14-0P 148579-44-6P 148579-49-1P 148579-54-8P 148579-69-5P
148579-71-9P 148579-75-3P **148579-77-5P** 148579-78-6P
148579-79-7P 148579-80-0P 148579-81-1P 148579-87-7P 148579-88-8P
148580-03-4P 148580-04-5P 148580-16-9P 160847-41-6P 160847-42-7P
160847-43-8P 160847-44-9P 160847-45-0P 160847-46-1P 160847-47-2P
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(prodrugs of anthracyclines for chemotherapy via enzyme-monoclonal antibody conjugates)

IT **148579-77-5P**
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(prodrugs of anthracyclines for chemotherapy via enzyme-monoclonal antibody conjugates)

RN 148579-77-5 HCAPLUS
CN α-D-Galactopyranoside, 2-(dibromomethyl)-4-nitrophenyl, 2,3,4,6-tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L43 ANSWER 14 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1992:105588 HCAPLUS
DOCUMENT NUMBER: 116:105588
TITLE: Chemoenzymic preparation of asymmetrized tris(hydroxymethyl)methane (THYM*) and of asymmetrized bis(hydroxymethyl)acetaldehyde (BHYMA*) as new highly versatile chiral building blocks
AUTHOR(S): Guanti, Giuseppe; Banfi, Luca; Narisano, Enrica
CORPORATE SOURCE: Ist. Chim. Org., CNR, Genoa, I-16132, Italy
SOURCE: Journal of Organic Chemistry (1992), 57(5), 1540-54
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 116:105588

AB A series of asymmetrized tris(hydroxymethyl)methane derivs., e.g., HOCH2CH(CH2OCH2Ph)CH2OSiMe2CMe3, and bis(hydroxymethyl)acetaldehyde derivs., e.g., PhCH2OCH2OCH2CH(CH2OSiMe2CMe3)CHO, were prepared in both enantiomeric forms through a chemoenzymic methodol. The key step is the highly enantioselective PPL-catalyzed monohydrolysis of (E)-2-alkenyl-1,3-diacetoxypropanes, e.g., PrCH:CHCH(CH2OAc)2. A careful study of the effect of unsatn. adjacent to the prochiral center in a series of 2-substituted 1,3-diacetoxypropanes confirmed the suggested beneficial effect of a π system in that position but also unveiled an unprecedented dramatic effect of the double-bond configuration on enantioselectivity. A new empirical model for the interpretation of these and other results, based both on polarity and steric arguments, is proposed. This study provides a general protocol for the efficient synthesis of asymmetrized 1,3-propanediols bearing saturated or unsatd. carbon chains in the position 2.

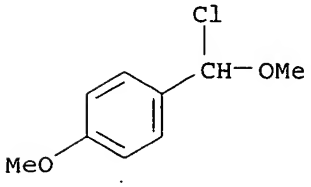
CC 23-14 (Aliphatic Compounds)
Section cross-reference(s): 7

IT **Enzymes**
RL: RCT (Reactant); RACT (Reactant or reagent)
(for asym. **hydrolysis** of alkenyldiacetoxypropanes)

IT 3587-60-8, Benzyl chloromethyl ether **64610-11-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkylation with, of alcs. in synthesis of bis- and tris(hydroxymethyl)-methanes)

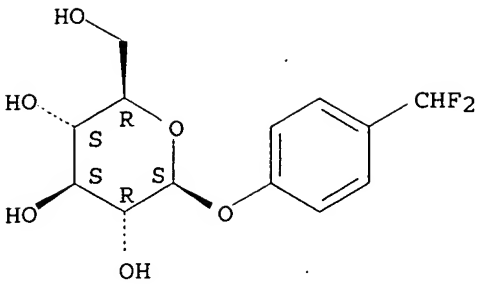
IT **64610-11-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkylation with, of alcs. in synthesis of bis- and

tris(hydroxymethyl)methanes)
RN 64610-11-3 HCAPLUS
CN Benzene, 1-(chloromethoxymethyl)-4-methoxy- (9CI) (CA INDEX NAME)



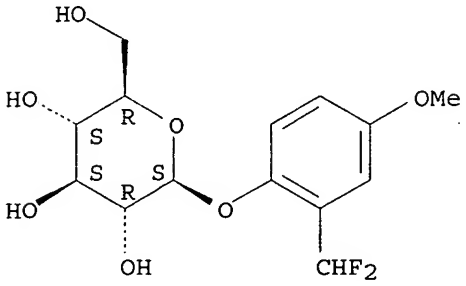
L43 ANSWER 15 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1991:38253 HCAPLUS
DOCUMENT NUMBER: 114:38253
TITLE: Ortho- and para-(difluoromethyl)aryl-β-D-glucosides: a new class of enzyme-activated irreversible inhibitors of β-glucosidases
AUTHOR(S): Halazy, S.; Berges, V.; Ehrhard, A.; Danzin, C.
CORPORATE SOURCE: Merrell Dow Res. Inst., Strasbourg, 67009, Fr.
SOURCE: Bioorganic Chemistry (1990), 18(3), 330-44
CODEN: BOCMBM; ISSN: 0045-2068
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 114:38253
AB New o- and p-(difluoromethyl)aryl-β-D-glucosides were stereoselectively prepared in 3 steps from 1-bromo-2,3,4,6-tetraacetyl glucose, using an appropriate o- or p-hydroxybenzaldehyde derivative The F atoms were introduced by reacting thus formed o- or p-O-glucosyl benzaldehyde derivs. with diethylaminosulfur trifluoride. The title compds. were potent time-dependent irreversible inhibitors of almond β-glucosidase. The inactivation was explained by the **enzyme**-catalyzed **hydrolysis** of the glucosidic linkage, releasing an o- or p-(difluoromethyl)phenol. The o- and p-(difluoromethyl)phenols were assumed to rapidly form fluorinated quinone methides which alkylated a nucleophilic residue of the enzyme active site.
CC 7-3 (Enzymes)
Section cross-reference(s): 33
IT **131497-36-4P** 131497-37-5P 131497-38-6P 131497-39-7P
131497-40-0P 131497-41-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and kinetics of glucosidase inhibition by)
IT **131497-36-4P 131497-40-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and kinetics of glucosidase inhibition by)
RN 131497-36-4 HCAPLUS
CN β-D-Glucopyranoside, 4-(difluoromethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.

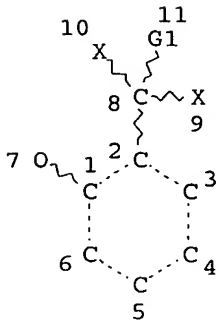


RN 131497-40-0 HCAPLUS
CN β-D-Glucopyranoside, 2-(difluoromethyl)-4-methoxyphenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> d que
L7 STR



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CONNECT IS E3 RC AT 4
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CONNECT IS E2 RC AT 6
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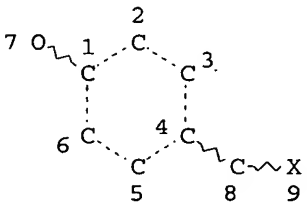
CONNECT IS E1 RC AT 12
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE
L9 3146 SEA FILE=REGISTRY SSS FUL L7
L15 STR



NODE ATTRIBUTES:
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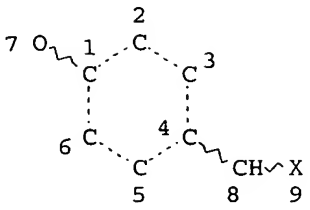
CONNECT IS E2 RC AT 7
CONNECT IS E3 RC AT 8
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE

L17 4953 SEA FILE=REGISTRY SSS FUL L15
L18 STR



NODE ATTRIBUTES:
CONNECT IS E2 RC AT 2
CONNECT IS E2 RC AT 3
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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE
L19 1145 SEA FILE=REGISTRY SUB=L17 SSS FUL L18
L20 4291 SEA FILE=REGISTRY ABB=ON PLU=ON L9 OR L19
L38 3528 SEA FILE=HCAPLUS ABB=ON PLU=ON ENZYMES+PFT/CT(L)HYDROL?
L39 27271 SEA FILE=HCAPLUS ABB=ON PLU=ON L38 OR HYDROL?(3A)?ENZYME?
L40 4 SEA FILE=HCAPLUS ABB=ON PLU=ON L39 AND L20
L41 169861 SEA FILE=HCAPLUS ABB=ON PLU=ON ENZYMES+PFT/CT
L42 12 SEA FILE=HCAPLUS ABB=ON PLU=ON L20 AND L41
L43 15 SEA FILE=HCAPLUS ABB=ON PLU=ON L40 OR L42
L45 10 SEA FILE=HCAPLUS ABB=ON PLU=ON L20(L)?ENZYM?
L46 6 SEA FILE=HCAPLUS ABB=ON PLU=ON L45 NOT L43

=> d l46 ibib abs hitind hitstr 1-6

L46 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:784629 HCAPLUS
DOCUMENT NUMBER: 139:292147
TITLE: Preparation of indole derivatives as phospholipase enzyme inhibitors
INVENTOR(S): Seehra, Jasbir S.; Kaila, Neelu; McKew, John C.; Bemis, Jean E.; Xiang, Yibin; Chen, Lihren
PATENT ASSIGNEE(S): Genetics Institute LLC, USA
SOURCE: U.S., 81 pp., Cont.-in-part of U.S. Ser. No. 30,102.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6630496	B1	20031007	US 2000-645042	20000824
BR 9909242	A	20001114	BR 1999-9242	19990217

PRIORITY APPLN. INFO.: US 1997-918400 B2 19970826

US 1998-30102 B2 19980225
WO 1999-IS3388 W 19990217

OTHER SOURCE(S): MARPAT 139:292147
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The indole derivs. (I), (II), and (III) [where A = CH2 or CH2CH2; B = (CH2)n, (CH2O)n, (CH2S)n, (OCH2)n, (SCH2)n, (CH=CH)n, (C.tplbond.C)n, CONR6, NR6CO, O, S, or NR6; R1 = H, OH, halo, etc.; R2, R3 = H, CO2H, alkyl, aryl, etc.; R4, R5 = H, OH, CN, CO2H, etc.; n = 0-4] and pharmaceutically acceptable salts thereof, were prepared Thus, 2,4-thiazolidinedione and K2CO3 followed by NaOH were added to 5-(benzyloxy)-1-(4-{[3,5-bis(trifluoromethyl)phenoxy]methyl}benzyl)-1H-indole-2-carboxaldehyde in EtOH to form the 2,4-thiazolidinedion-4-ylidene derivative The ylidene was dissolved in a solution of DMF and NaH, reacted with an alkyl ester of 4-(bromomethyl)benzoic acid, and deesterified with HF to yield the acid, (E)-(IV). The title compds. are useful as phospholipase enzyme inhibitors, especially cytosolic phospholipase A2 (cPLA2), for treatment of inflammatory conditions and pain, particularly where inhibition of production of prostaglandins, leukotrienes, and PAF are all desired. Eighty-seven compds. of the invention were tested for phospholipase enzyme inhibiting activity in the LysoPC and/or Coumarine assay. IC50 values ranged from 0.081 μM to >50 μM for the LysoPC assay and from 2.5 μM to >64 μM for the Coumarine assay. Selected compds. were tested for in vivo activity in the carrageenan-induced rat paw edema test, and showed 4.2% to 34.2% inhibition. Forty-eight compds. of the invention were tested for cPLA2 enzyme activity, and exhibited 25% to 95% inhibition at concns. of 3 μM to 100 μM. Pharmaceutical composition comprising the compound I was claimed.

IC ICM C07D417-06
ICS A61K031-404; A61K031-427

NCL 514369000; 548181000; 548183000

CC 27-11 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 63

IT

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204016-36-4P	204016-37-5P	204016-38-6P	204016-39-7P	
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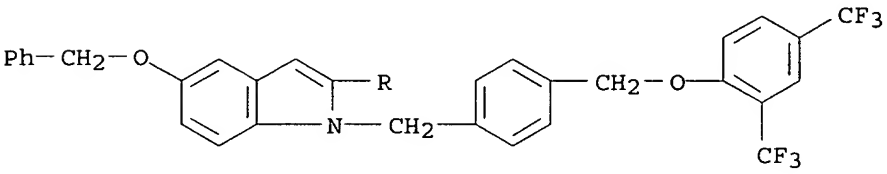
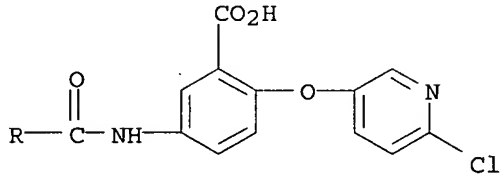
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of indole derivs. as phospholipase **enzyme** inhibitors for treatment of inflammatory conditions)

IT **204016-36-4P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of indole derivs. as phospholipase **enzyme** inhibitors for treatment of inflammatory conditions)

RN 204016-36-4 HCAPLUS
CN Benzoic acid, 5-[[[1-[[4-[[2,4-bis(trifluoromethyl)phenoxy]methyl]phenyl]methyl]-5-(phenylmethoxy)-1H-indol-2-yl]carbonyl]amino]-2-[(6-chloro-3-pyridinyl)oxy]- (9CI) (CA INDEX NAME)





REFERENCE COUNT: 70 THERE ARE 70 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L46 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:566043 HCAPLUS
DOCUMENT NUMBER: 131:199620
TITLE: Preparation of indole derivatives as phospholipase enzyme inhibitors
INVENTOR(S): Seehra, Jasbir S.; Xiang, Yibin; Bemis, Jean; McKew, John; Kaila, Neelu; Chen, Lihren
PATENT ASSIGNEE(S): Genetics Institute, Inc., USA
SOURCE: PCT Int. Appl., 225 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9943672	A1	19990902	WO 1999-US3388	19990217
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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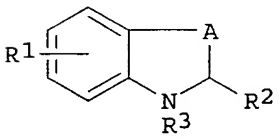
AU 9932970	A1	19990915	AU 1999-32970	19990217
BR 9909242	A	20001114	BR 1999-9242	19990217
TR 200002445	T2	20001221	TR 2000-200002445	19990217
EP 1062216	A1	20001227	EP 1999-936073	19990217
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
JP 2002504551	T2	20020212	JP 2000-533428	19990217
EE 200000522	A	20020215	EE 2000-522	19990217
HR 2000000513	A1	20011231	HR 2000-513	20000731
NO 2000004217	A	20001023	NO 2000-4217	20000823
BG 104781	A	20011031	BG 2000-104781	20000919
PRIORITY APPLN. INFO.:			US 1998-30102 A	19980225
			WO 1999-IS3388 W	19990217
			WO 1999-US3388 W	19990217

OTHER SOURCE(S): MARPAT 131:199620

GI



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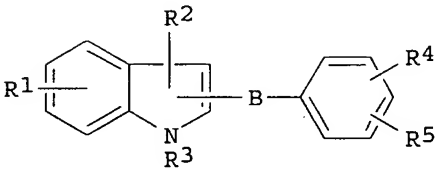

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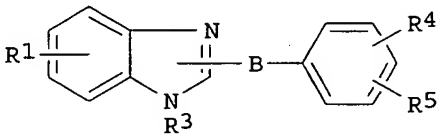

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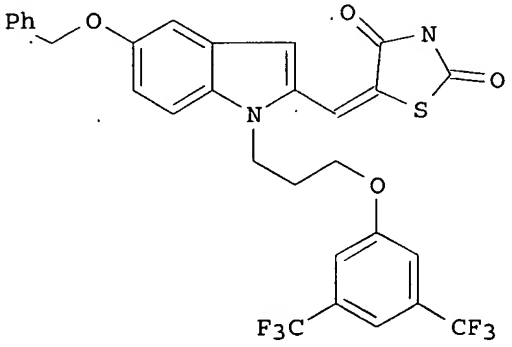

IV

AB Indole derivs. (I), (II), and (III) [where A = CH2 or CH2CH2; B = (CH2)n, (CH2O)n, (CH2S)n, (OCH2)n, (SCH2)n, (CH=CH)n, (C.tplbond.C)n, CON(R6), N(R6)CO, O, S, or N(R6); R1 and R5 = independently H, OH, halogen, CN, NO2, C1-5 alkyl, alkenyl, alkynyl, or (un)substituted aryl, etc.; R2 and R3 = independently H, CO2H, COR5, CONR5R6, (CH2)nW(CH2)mZR5, (CH2)nWR5, ZR5, C1-10 alkyl, alkenyl, or substituted aryl; R4 = H, OH, OR6, SR6, CN, COR6, NHR6, CO2H, COR6R7, NO2, (un)substituted sulfamidocarbonyl, C1-5 alkyl, alkenyl, or substituted aryl; R6, R7 = H, C1-5 alkyl, alkenyl, alkynyl, or (un)substituted aryl; W = O, S, CH2, CH=CH, C.tplbond.C, or N(R6); X = O, S, N(R6); Z = CH2, O, S, N(R6), CO, CON(R6), N(R6)CO; m and n = independently 0-4] and pharmaceutically acceptable salts thereof, were prepared Thus, 2,4-thiazolidinedione and K2CO3 followed by NaOH were added to 5-(benzyloxyl)-1-(4-{[3,5-bis(trifluoromethyl)phenoxy]methyl}benzyl)-1H-indole-2-carboxaldehyde in EtOH to form the 2,4-thiazolidinedion-4-ylidene derivative The ylidene was dissolved in a solution of DMF and NaH, reacted with
an alkyl ester of 4-(bromomethyl)benzoic acid, and deesterified with HF to yield the acid, (E)-(IV). The title compds. are useful as phospholipase enzyme inhibitors, especially cytosolic phospholipase A2 (cPLA2), for treatment of inflammatory conditions, particularly where inhibition of production of prostaglandins, leukotrienes, and PAF are all desired. Eighty-seven compds. of the invention were tested for phospholipase enzyme inhibiting activity in the LysoPC and/or Coumarine assay. IC50 values ranged from 0.081 μM to >50 μM for the LysoPC assay and from 2.5 μM to >64 μM for the Coumarine assay. Selected compds. were tested for in vivo activity in the carrageenan-induced rat paw edema test, and showed 4.2% to 34.2% inhibition. Forty-eight compds. of the invention were tested for cPLA2 enzyme activity, and exhibited 25% to 95% inhibition at concns. of 3 μM to 100 μM.

IC ICM C07D417-06
ICS A61K031-40; C07D409-04; C07D401-12; C07D403-04; C07D209-22; C07D209-12; C07D209-10; C07D401-06; C07D209-42; C07D209-14; C07D403-06; C07D405-04; C07D417-10; C07D405-12

CC 27-11 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 63

IT

204016-27-3P	204016-28-4P	204016-29-5P	204016-30-8P	204016-31-9P
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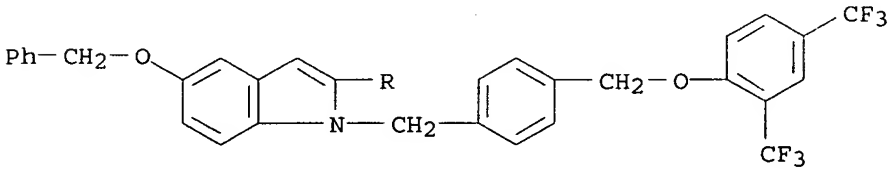
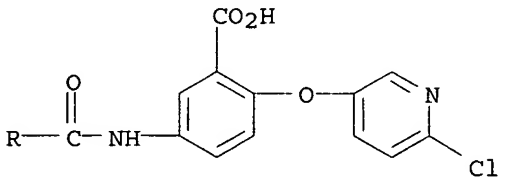
241489-90-7P 241489-91-8P 241489-92-9P 241489-93-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of indole derivs. as phospholipase **enzyme** inhibitors for treatment of inflammatory conditions)

IT **204016-36-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of indole derivs. as phospholipase **enzyme** inhibitors for treatment of inflammatory conditions)

RN 204016-36-4 HCAPLUS
CN Benzoic acid, 5-[[[1-[[4-[[2,4-bis(trifluoromethyl)phenoxy]methyl]phenyl]methyl]-5-(phenylmethoxy)-1H-indol-2-yl]carbonyl]amino]-2-[(6-chloro-3-pyridinyl)oxy]- (9CI) (CA INDEX NAME)





REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L46 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:163566 HCAPLUS
DOCUMENT NUMBER: 128:204806
TITLE: Preparation of indole derivatives as phospholipase enzyme inhibitors
INVENTOR(S): Xiang, Yibin; Bemis, Jean; McKew, John; Kaila, Neelu
PATENT ASSIGNEE(S): Genetics Institute, Inc., USA
SOURCE: PCT Int. Appl., 115 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

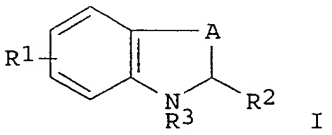
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9808818	A1	19980305	WO 1997-US14943	19970826

W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ,

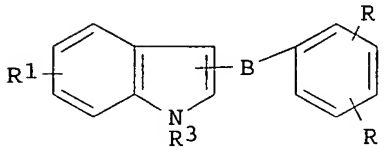
LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

CA 2264020	AA	19980305	CA 1997-2264020		19970826
AU 9740882	A1	19980319	AU 1997-40882		19970826
AU 717430	B2	20000323			
EP 922028	A1	19990616	EP 1997-938589		19970826
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI					
JP 2000516958	T2	20001219	JP 1998-511798		19970826
PRIORITY APPLN. INFO.:			US 1996-703115	A	19960826
			WO 1997-US14943	W	19970826

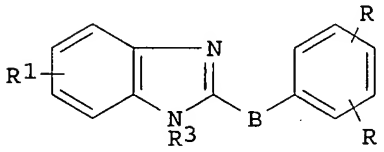
OTHER SOURCE(S): MARPAT 128:204806
GI



I



II



III

AB Title compds. I, II, III (A is independent of any other group and is selected from the group consisting of -CH2- and -CH2-CH2-; B is independent of any other group and is selected from the group consisting of -(CH2)n-, -(CH2O)n-, -(CH2S)n-, -(OCH2)n-, -(SCH2)n-, -(CH=CH)n-, -(C.tplbond.C)n-, -CON(R6)-, -N(R6)CO-, -O-, -S- and -N(R6)-; R2 is independent of any other R group and is selected from the group consisting of -H, -COOH, -COR5, -CONR5R6, -(CH2)n-W-(CH2)m-Z-R5, -(CH2)n-W-R5, -Z-R5, C1-C10 alkyl, alkenyl and substituted aryl; R3 is independent of any other R group and is selected from the group consisting of -H, -COOH, -COR5, -CONR5R6, -(CH2)n-W-(CH2)m-Z-R5, -(CH2)n-W-R5, -Z-R5 wherein:, C1-C10 alkyl, alkenyl and substituted aryl) and a pharmaceutically acceptable salt thereof; which inhibit the activity of phospholipase enzymes, particularly cytosolic phospholipase A2 were prepared Pharmaceutical compns. comprising such compds. and methods of treatment using such compns. are also disclosed.

IC ICM C07D209-12
ICS A61K031-40; C07D209-42; C07D401-12; C07D209-10; C07D405-12

CC 27-11 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 1, 63

IT 204016-27-3P 204016-28-4P 204016-29-5P 204016-30-8P 204016-31-9P
204016-32-0P 204016-33-1P 204016-34-2P 204016-35-3P
204016-36-4P 204016-37-5P 204016-38-6P 204016-39-7P
204016-40-0P 204016-41-1P 204016-42-2P 204016-43-3P 204016-44-4P
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204016-60-4P 204016-61-5P 204016-62-6P 204016-63-7P 204016-64-8P
204016-65-9P 204016-66-0P 204016-67-1P 204016-68-2P 204016-69-3P
204016-70-6P 204016-71-7P 204016-72-8P 204016-73-9P 204016-74-0P
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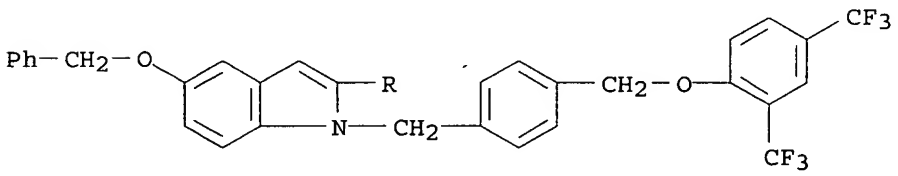
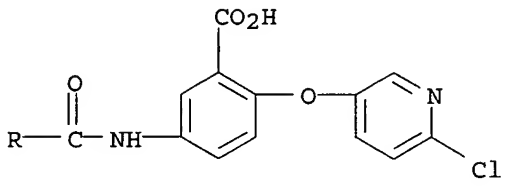
204017-10-7P 204017-11-8P 204017-12-9P 204017-13-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of indole derivs. as phospholipase **enzyme** inhibitors)

IT **204016-36-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of indole derivs. as phospholipase **enzyme** inhibitors)

RN 204016-36-4 HCAPLUS

CN Benzoic acid, 5-[[[1-[[4-[[2,4-bis(trifluoromethyl)phenoxy]methyl]phenyl]methyl]-5-(phenylmethoxy)-1H-indol-2-yl]carbonyl]amino]-2-[(6-chloro-3-pyridinyl)oxy]- (9CI) (CA INDEX NAME)





REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

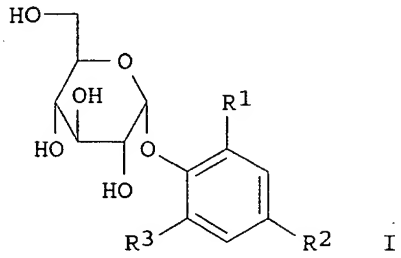
L46 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:317204 HCAPLUS
DOCUMENT NUMBER: 122:187904
TITLE: (Halogenomethyl)phenyl α-D-glucopyranosides as enzyme-activated irreversible inhibitors of yeast

α-glucosidase and potential anti-HIV agents

AUTHOR(S): Briggs, Josie C.; Haines, Alan H.; Taylor, Richard J. K.
CORPORATE SOURCE: School Chem. Sciences, Univ. East Anglia, Norwich, NR4 7TJ, UK

SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1995), (1), 27-32
CODEN: JCPRB4; ISSN: 0300-922X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

GI



I

AB A range of (halogenomethyl)phenyl α-D-glucopyranosides I (R1 = CH2Cl, CH2F, R2 = R3 = H; R1 = R3 = H, R2 = NO2, CH2Cl; R1 = CHCl2, CH2Cl, R2 = NO2, R3 = H), prepared from corresponding methylphenyl glucosides by synthetic manipulation of the aglycon moiety, have been investigated as enzyme-activated irreversible inhibitors of yeast α-glucosidase and their anti-HIV activity measured. Compds. I, which also contain a 4- and 6-nitro group in the Ph ring of the aglycon, are much more effective inhibitors of the enzyme than are compds. which lack this feature.

CC 33-3 (Carbohydrates)
Section cross-reference(s): 1, 7

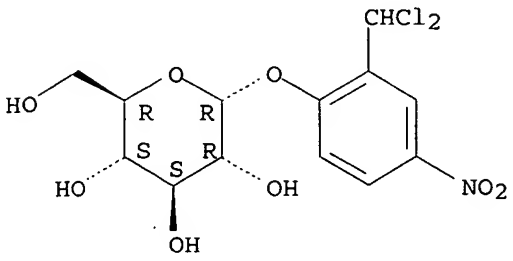
IT 143836-10-6P 143836-15-1P 161767-40-4P 161767-41-5P
161767-42-6P 161767-43-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(halomethylphenyl adglucopyranosides as **enzyme**-activated irreversible inhibitors of yeast aglucosidase and potential anti-HIV agents)

IT 32742-30-6P 78617-45-5P 143836-11-7P 143836-12-8P 143836-13-9P
161767-44-8P 161767-45-9P 161767-46-0P 161767-47-1P 161767-48-2P
161767-49-3P 161767-50-6P **161767-51-7P** 161767-52-8P
161767-53-9P 161767-54-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(halomethylphenyl adglucopyranosides as **enzyme**-activated irreversible inhibitors of yeast aglucosidase and potential anti-HIV agents)

IT **161767-42-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(halomethylphenyl adglucopyranosides as **enzyme**-activated

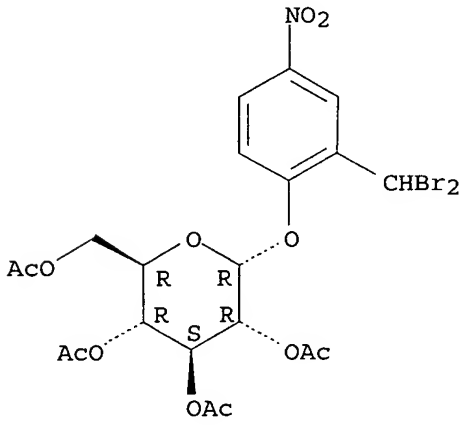
irreversible inhibitors of yeast aglucosidase and potential anti-HIV agents)
RN 161767-42-6 HCAPLUS
CN α-D-Glucopyranoside, 2-(dichloromethyl)-4-nitrophenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



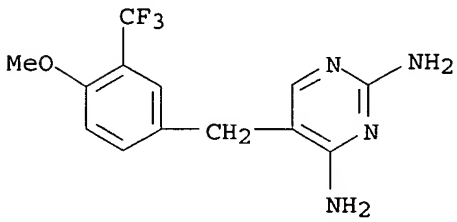
IT **161767-51-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(halomethylphenyl adglucopyranosides as **enzyme**-activated irreversible inhibitors of yeast aglucosidase and potential anti-HIV agents)
RN 161767-51-7 HCAPLUS
CN α-D-Glucopyranoside, 2-(dibromomethyl)-4-nitrophenyl, 2,3,4,6-tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

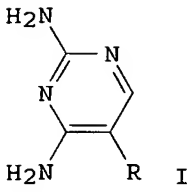


L46 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1985:91923 HCAPLUS
DOCUMENT NUMBER: 102:91923
TITLE: Use of physicochemical parameters in distance geometry and related three-dimensional quantitative structure-activity relationships: A demonstration using Escherichia coli dihydrofolate reductase inhibitors
AUTHOR(S): Ghose, Arup K.; Crippen, Gordon M.
CORPORATE SOURCE: Dep. Chem., Texas A and M Univ., College Station, TX,

77843, USA
SOURCE: Journal of Medicinal Chemistry (1985), 28(3), 333-46
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A method for using physicochem. parameters in distance geometry or comparable 3-dimensional QSAR is described. A 3-dimensional receptor model for E. coli dihydrofolate reductase was developed from inhibition data of 25 pyrimidines and 14 triazines. The model successfully predicted the binding sites of 5 pyrimidines and 5 triazines. The greatest advantage of the method is that x-ray data and 3-dimensional mol. graphics can be used directly.
CC 7-3 (Enzymes)
Section cross-reference(s): 1
IT 640-02-8 738-70-5 1492-81-5 3977-24-0 4022-58-6 4038-62-4
4653-78-5 5355-16-8 7319-45-1 13344-99-5 13351-02-5 14484-50-5
17711-73-8 17740-28-2 17740-29-3 18588-43-7 20285-70-5
20344-69-8 46726-70-9 49561-94-6 50823-94-4 **50823-96-6**
59481-28-6 69945-50-2 69945-51-3 69945-52-4 69945-53-5
69945-55-7 69945-56-8 69945-58-0 69945-59-1 71525-05-8
77113-54-3 77113-55-4 77113-56-5 77113-57-6 77113-58-7
94295-02-0 94295-03-1
RL: BIOL (Biological study)
(dihydrofolate reductase inhibition by, **enzyme** model in relation to)
IT **50823-96-6**
RL: BIOL (Biological study)
(dihydrofolate reductase inhibition by, **enzyme** model in relation to)
RN 50823-96-6 HCAPLUS
CN 2,4-Pyrimidinediamine, 5-[[4-methoxy-3-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)



L46 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1982:115502 HCAPLUS
DOCUMENT NUMBER: 96:115502
TITLE: A comparison of the inhibitory action of 5-(substituted-benzyl)-2,4-diaminopyrimidines on dihydrofolate reductase from chicken liver with that from bovine liver
AUTHOR(S): Li, Ren Li; Hansch, Corwin; Kaufman, Bernard T.
CORPORATE SOURCE: Dep. Chem., Pomona Coll., Claremont, CA, 91711, USA
SOURCE: Journal of Medicinal Chemistry (1982), 25(4), 435-40
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB Forty-four 5-(substituted-benzyl)-2,4-diaminopyrimidines I (R = substituted benzyl) were synthesized and tested as inhibitors of chicken and bovine liver dihydrofolate reductase [9002-03-3]. The chicken **enzyme** is, on the average, about 10 times less easily inhibited than bovine **enzyme**. Compds. which show the greatest selectivity are I [R = CH2C6H4NHCOMe-4 [69945-53-5], CH2C6H4I-3 [30077-60-2], CH2C6H4O(CH2)3Me [77113-59-8], CH2C6H3(CF3)OMe-3,4 [**50823-96-6**], and CH2C6H2(OMe)3-3,4,5 [738-70-5]]. The inhibition consts. were used to formulate QSAR for comparative purposes.

CC 1-3 (Pharmacology)
Section cross-reference(s): 7, 22, 28